

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041323\
 Data File : VX035041.D
 Acq On : 12 Apr 2023 13:02
 Operator : JC/MD
 Sample : 02268-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 50002-TOTE

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\82X032923W.M
 Title : SW846 8260

Signal : TIC: VX035041.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	19	rVB	100030	94247	6.31%	0.271%
2	1.355	40	44	50	rBV2	52437	65243	4.37%	0.188%
3	1.453	57	60	65	rBV	58176	69112	4.63%	0.199%
4	2.392	206	214	229	rVB	429411	891011	59.70%	2.566%
5	2.599	237	248	262	rBV2	26280	145948	9.78%	0.420%
6	2.995	299	313	337	rVB3	29816	144292	9.67%	0.416%
7	4.233	504	516	524	rBV3	29751	90565	6.07%	0.261%
8	4.562	561	570	590	rBV	143636	432670	28.99%	1.246%
9	5.093	639	657	678	rBV5	16662	99829	6.69%	0.287%
10	5.385	694	705	718	rBV	157078	462750	31.01%	1.333%
11	5.550	721	732	753	rVB	281064	805102	53.95%	2.318%
12	5.958	788	799	808	rBV	181803	494589	33.14%	1.424%
13	6.635	896	910	921	rBV	410661	1074701	72.01%	3.095%
14	6.763	921	931	947	rVB	446789	1078561	72.27%	3.106%
15	6.952	954	962	978	rBV	185566	445318	29.84%	1.282%
16	7.245	1002	1010	1028	rBV3	57677	225373	15.10%	0.649%
17	7.458	1038	1045	1059	rVV2	258168	620898	41.60%	1.788%
18	7.580	1059	1065	1070	rVV	53860	113042	7.57%	0.326%
19	7.641	1070	1075	1092	rVB	55664	115477	7.74%	0.333%
20	7.903	1112	1118	1135	rVB2	105997	247426	16.58%	0.713%
21	8.574	1223	1228	1233	rVV	175439	281774	18.88%	0.811%
22	8.647	1233	1240	1246	rVV	922466	1492434	100.00%	4.298%
23	8.714	1246	1251	1258	rVV2	264421	463816	31.08%	1.336%
24	8.805	1260	1266	1282	rVB	248984	425272	28.50%	1.225%
25	8.939	1282	1288	1295	rBV	70610	107535	7.21%	0.310%
26	9.238	1332	1337	1345	rBV	221118	365977	24.52%	1.054%
27	9.311	1345	1349	1356	rVB	61349	87957	5.89%	0.253%
28	9.433	1363	1369	1375	rBV2	178403	306455	20.53%	0.883%
29	9.519	1375	1383	1397	rVV	241789	399654	26.78%	1.151%
30	9.702	1407	1413	1419	rVB2	55262	123060	8.25%	0.354%
31	9.836	1431	1435	1442	rVB	131058	178413	11.95%	0.514%
32	9.945	1448	1453	1461	rBV	164295	247324	16.57%	0.712%
33	10.055	1461	1471	1476	rVV	917861	1369002	91.73%	3.942%
34	10.214	1488	1497	1503	rBV2	511343	940707	63.03%	2.709%
35	10.268	1503	1506	1508	rVV	156914	218599	14.65%	0.630%
36	10.299	1508	1511	1518	rVB	682704	886206	59.38%	2.552%

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37	10.384	1518	1525	1529	rBV2	43907	85089	5.70%	0.245%
38	10.506	1538	1545	1549	rBV2	44978	67351	4.51%	0.194%
39	10.640	1562	1567	1572	rVV	430722	563802	37.78%	1.624%
40	10.683	1572	1574	1579	rVB2	53593	63175	4.23%	0.182%
41	10.768	1581	1588	1595	rBV	178184	257308	17.24%	0.741%
42	10.890	1599	1608	1614	rBV2	136349	353985	23.72%	1.019%
43	10.963	1614	1620	1624	rVB3	58787	115800	7.76%	0.333%
44	11.012	1624	1628	1634	rBV	51778	74578	5.00%	0.215%
45	11.079	1634	1639	1650	rBV2	727435	1108357	74.27%	3.192%
46	11.177	1650	1655	1660	rVB4	55332	95302	6.39%	0.274%
47	11.232	1660	1664	1668	rBV2	45726	68515	4.59%	0.197%
48	11.305	1668	1676	1679	rBV2	134259	209646	14.05%	0.604%
49	11.378	1679	1688	1696	rBV2	432251	823636	55.19%	2.372%
50	11.451	1696	1700	1710	rVB3	265910	490171	32.84%	1.412%
51	11.573	1716	1720	1723	rBV	164483	208024	13.94%	0.599%
52	11.616	1723	1727	1736	rVB2	359083	512655	34.35%	1.476%
53	11.695	1736	1740	1742	rBV	51076	69523	4.66%	0.200%
54	11.750	1742	1749	1755	rVB	1057652	1381587	92.57%	3.979%
55	11.835	1758	1763	1769	rVB2	195007	300564	20.14%	0.866%
56	11.902	1769	1774	1779	rBV4	52799	92886	6.22%	0.267%
57	11.969	1781	1785	1789	rBV	415981	553075	37.06%	1.593%
58	12.024	1789	1794	1800	rVB	833268	1081372	72.46%	3.114%
59	12.085	1800	1804	1808	rBV	393122	478768	32.08%	1.379%
60	12.244	1823	1830	1838	rVB2	480940	780175	52.28%	2.247%
61	12.317	1838	1842	1853	rBV5	193566	429421	28.77%	1.237%
62	12.421	1853	1859	1863	rBV3	119677	177057	11.86%	0.510%
63	12.463	1863	1866	1872	rVB	107593	143055	9.59%	0.412%
64	12.530	1872	1877	1879	rBV	132851	180424	12.09%	0.520%
65	12.555	1879	1881	1885	rVB	109773	109173	7.32%	0.314%
66	12.610	1885	1890	1893	rBV	160485	209234	14.02%	0.603%
67	12.646	1893	1896	1900	rVB	73148	87168	5.84%	0.251%
68	12.701	1900	1905	1913	rVB2	170056	297411	19.93%	0.856%
69	12.805	1918	1922	1926	rBV3	36206	61344	4.11%	0.177%
70	12.847	1926	1929	1933	rVB	66591	76850	5.15%	0.221%
71	12.920	1933	1941	1944	rBV	123758	163553	10.96%	0.471%
72	12.963	1944	1948	1953	rVB	204752	251518	16.85%	0.724%
73	13.024	1953	1958	1959	rBV3	42842	67969	4.55%	0.196%
74	13.170	1978	1982	1985	rVB	241356	291123	19.51%	0.838%
75	13.292	1991	2002	2007	rBV3	601241	957797	64.18%	2.758%
76	13.341	2007	2010	2013	rBV3	88945	93222	6.25%	0.268%

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77	13.420	2019	2023	2032	rVB	532045	716803	48.03%	2.064%
78	13.506	2032	2037	2040	rBV2	46050	68841	4.61%	0.198%
79	13.542	2040	2043	2046	rBV	81449	100052	6.70%	0.288%
80	13.585	2046	2050	2054	rBV3	92157	158933	10.65%	0.458%
81	13.664	2060	2063	2071	rVB3	84003	122590	8.21%	0.353%
82	13.774	2077	2081	2088	rVB	801898	984028	65.93%	2.834%
83	13.853	2088	2094	2100	rVB4	126376	217559	14.58%	0.627%
84	13.926	2101	2106	2110	rBV2	120177	163640	10.96%	0.471%
85	14.036	2121	2124	2127	rVV	129563	133449	8.94%	0.384%
86	14.079	2127	2131	2137	rVB	85316	117094	7.85%	0.337%
87	14.231	2150	2156	2159	rBV	279440	427529	28.65%	1.231%
88	14.371	2175	2179	2183	rBV	100448	118377	7.93%	0.341%
89	14.481	2192	2197	2207	rBV2	198848	311819	20.89%	0.898%
90	14.640	2215	2223	2226	rBV	391262	613901	41.13%	1.768%
91	14.670	2226	2228	2233	rVB2	51579	63370	4.25%	0.182%
92	14.755	2239	2242	2243	rBV	124034	122011	8.18%	0.351%
93	14.780	2243	2246	2250	rVB	301561	370190	24.80%	1.066%
94	15.182	2308	2312	2314	rBV2	65408	88393	5.92%	0.255%
95	15.207	2314	2316	2320	rVB	75967	90987	6.10%	0.262%
96	15.487	2356	2362	2373	rVB3	135891	250723	16.80%	0.722%
97	15.615	2378	2383	2386	rVV	98992	167475	11.22%	0.482%
98	15.652	2386	2389	2395	rVB	55380	87934	5.89%	0.253%
99	16.322	2495	2499	2504	rBV2	54328	100573	6.74%	0.290%
100	16.377	2504	2508	2513	rVB	52191	87161	5.84%	0.251%

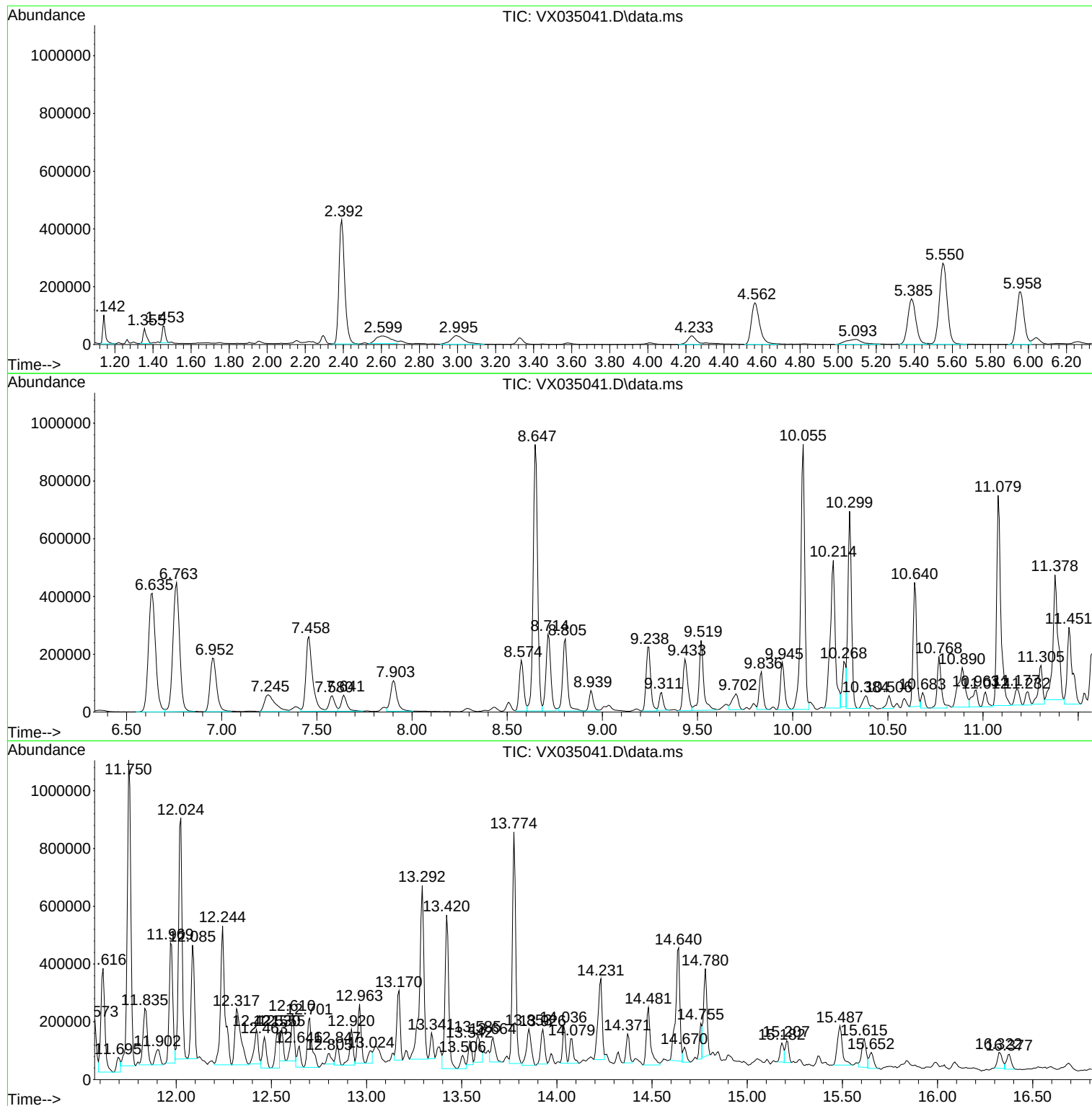
Sum of corrected areas: 34725434

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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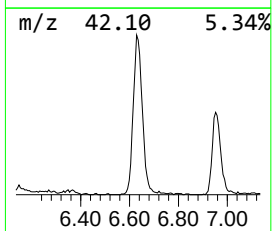
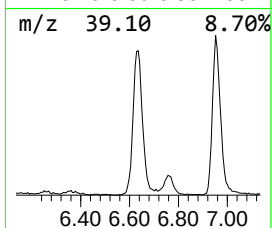
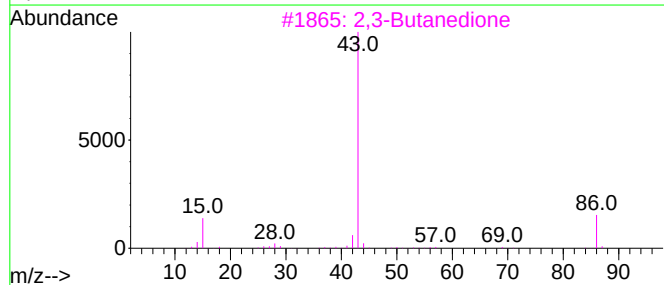
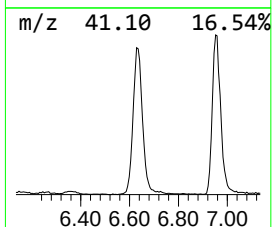
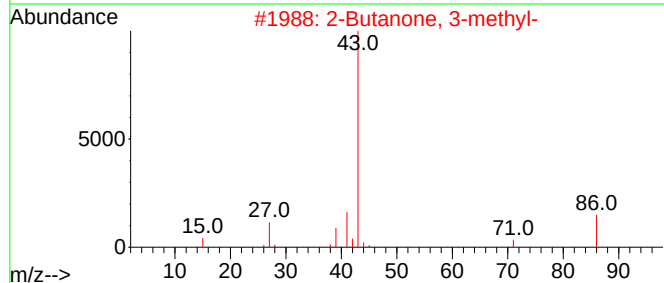
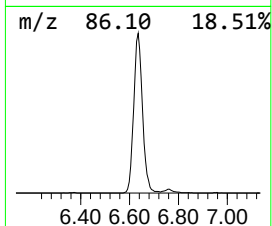
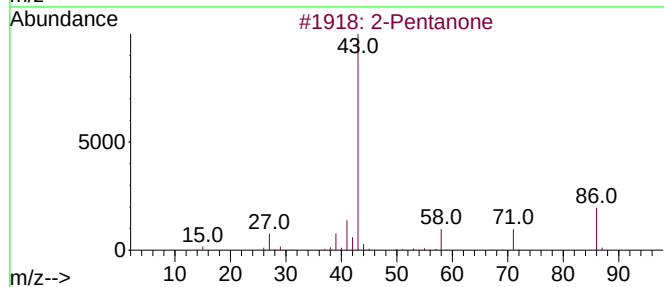
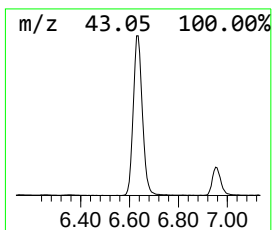
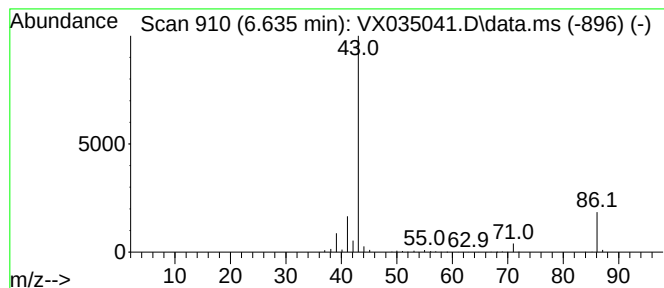
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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

Peak Number 1 2-Pentanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.635	49.82 ug/l	1074700	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone			86	C5H10O	000107-87-9	72
2	2-Butanone, 3-methyl-			86	C5H10O	000563-80-4	72
3	2,3-Butanedione			86	C4H6O2	000431-03-8	53
4	3,3-Dimethyl-2,4-pentane dione			128	C7H12O2	003142-58-3	36
5	3-Aminopyrrolidine			86	C4H10N2	079286-79-6	9



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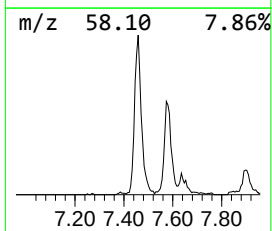
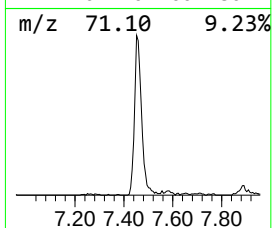
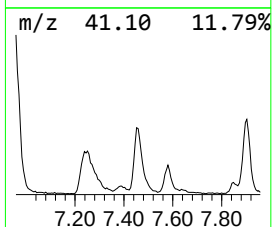
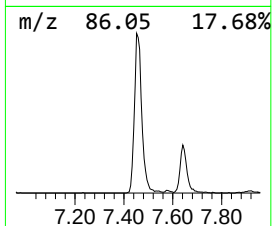
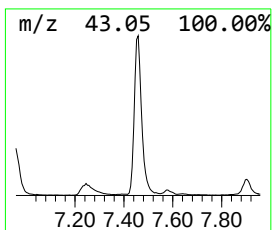
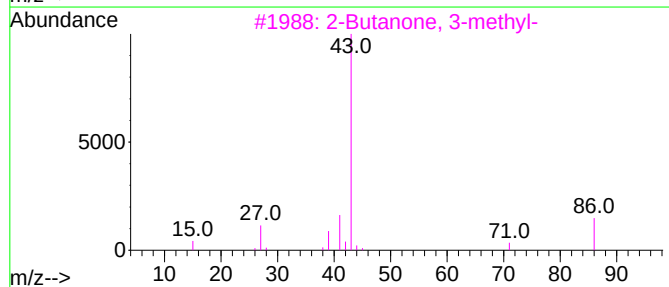
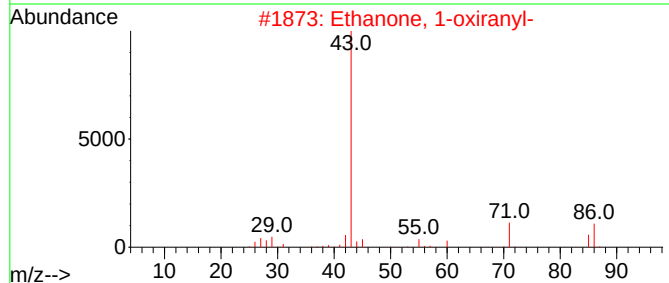
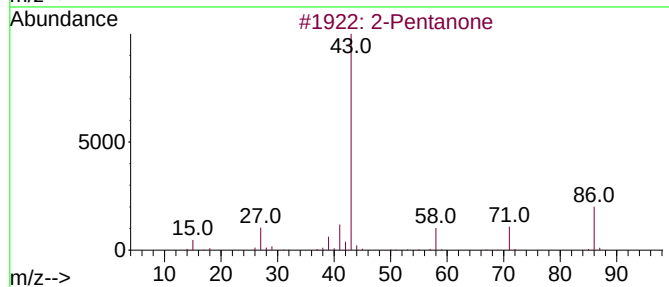
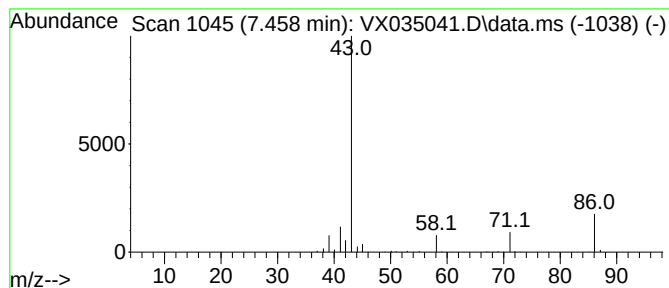
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanone, 1-oxiranyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.458	28.78 ug/l	620898	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone	86	C5H10O	000107-87-9	86
2		Ethanone, 1-oxiranyl-	86	C4H6O2	004401-11-0	64
3		2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	59
4		2,3-Butanedione	86	C4H6O2	000431-03-8	47
5		3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	33



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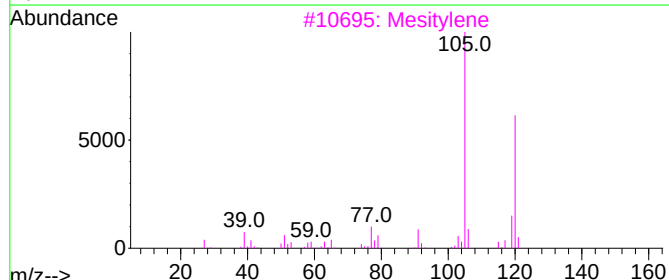
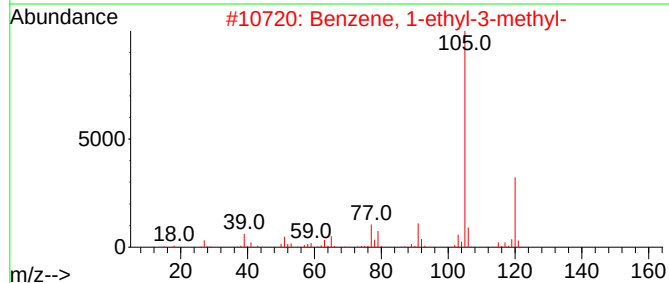
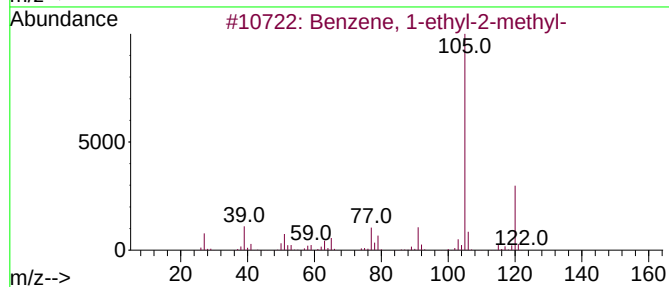
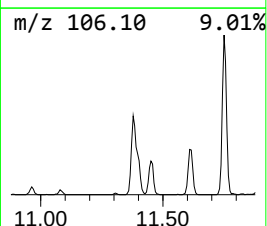
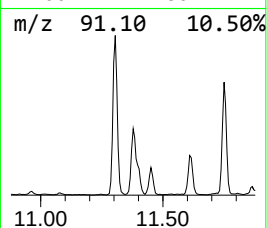
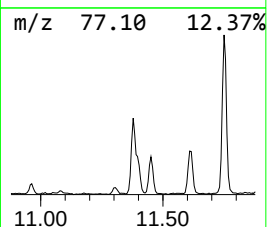
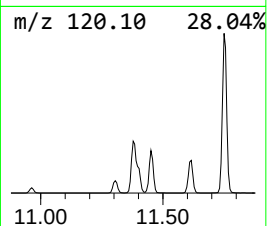
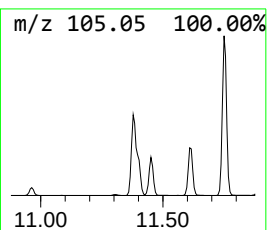
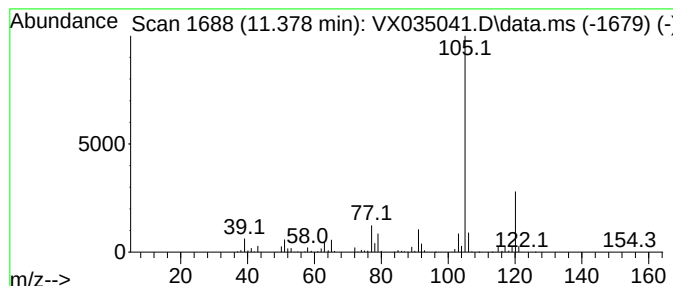
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Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	38.08 ug/l	823636	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	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041323\
Data File : VX035041.D
Acq On : 12 Apr 2023 13:02
Operator : JC/MD
Sample : 02268-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50002-TOTE

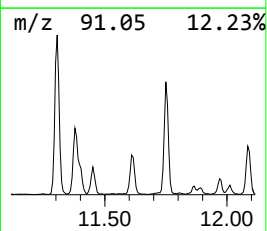
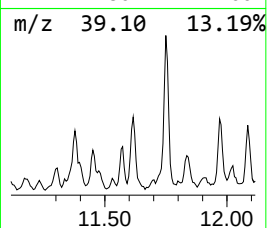
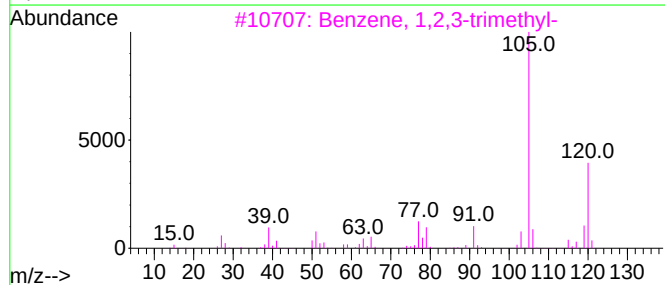
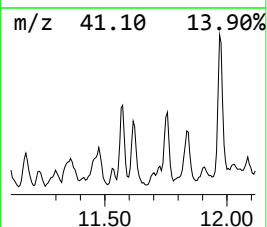
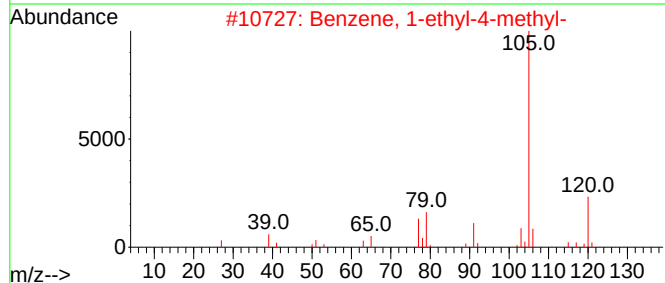
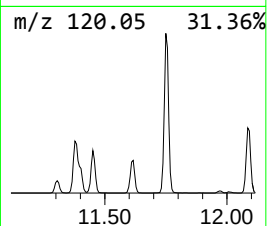
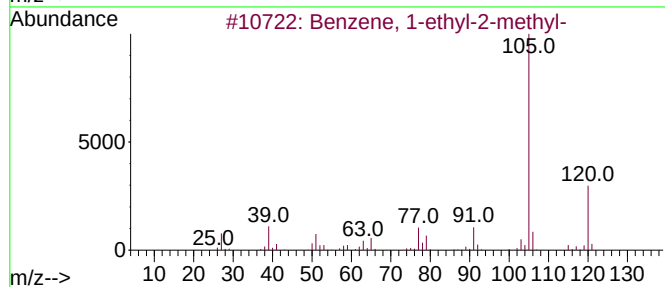
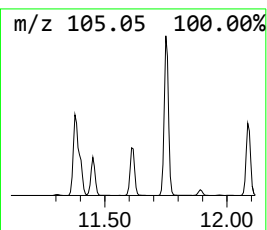
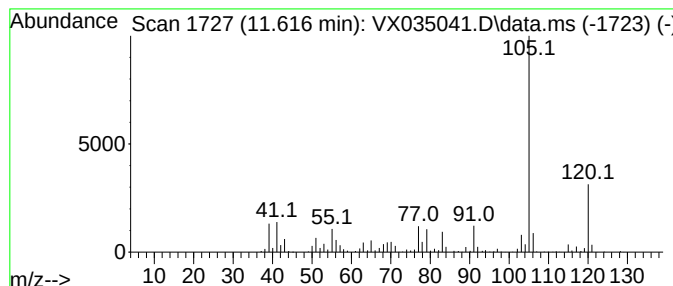
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Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-ethyl-4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	23.70 ug/l	512655	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	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Mesitylene	120	C9H12	000108-67-8	90
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041323\
Data File : VX035041.D
Acq On : 12 Apr 2023 13:02
Operator : JC/MD
Sample : 02268-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50002-TOTE

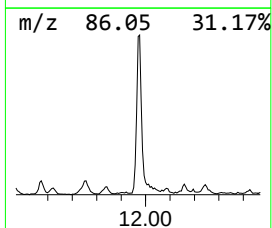
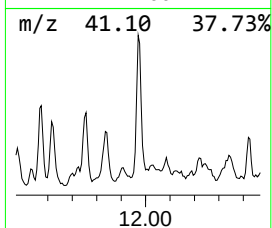
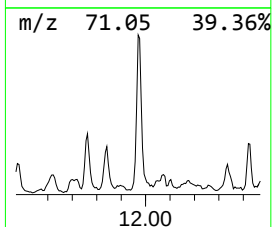
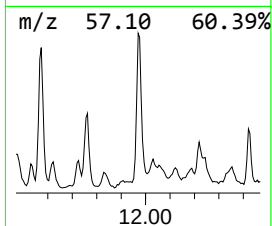
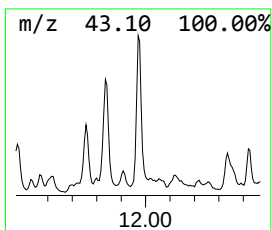
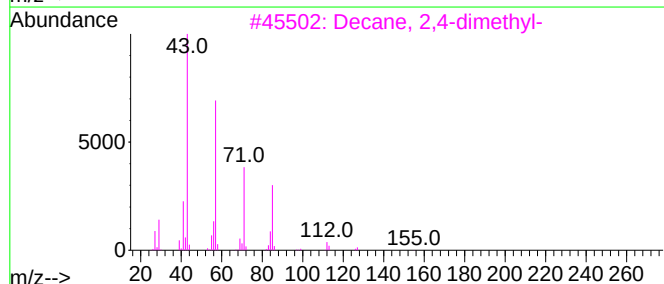
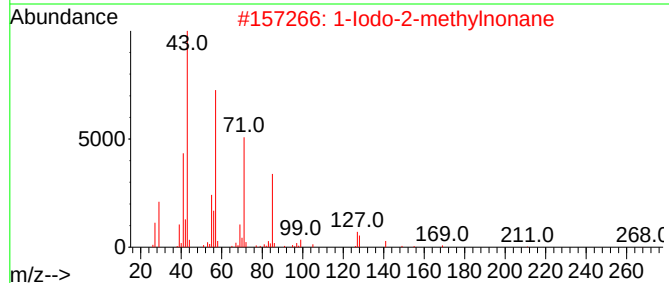
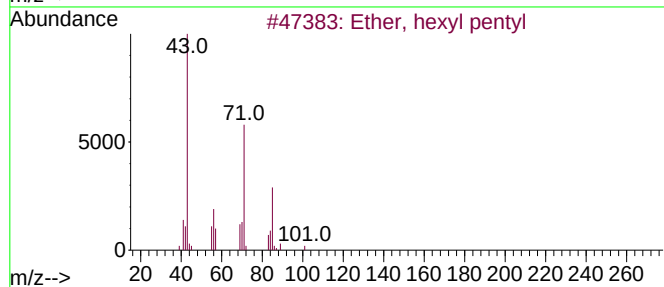
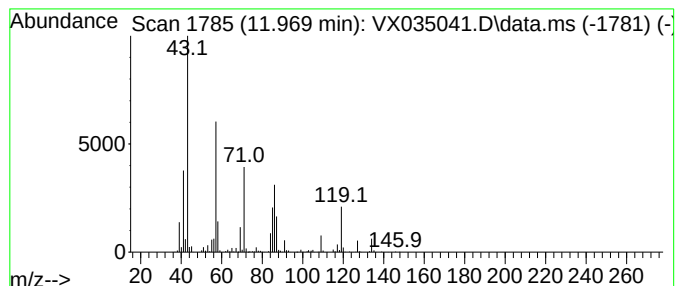
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Quant Title : SW846 8260

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

Peak Number 5 unknown11.969 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	25.57 ug/l	553075	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ether, hexyl pentyl	172	C11H24O	032357-83-8	38
2			1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	32
3			Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	32
4			Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3	32
5			Sulfurous acid, nonyl 2-propyl e...	250	C12H26O3S	1000309-12-0	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041323\
Data File : VX035041.D
Acq On : 12 Apr 2023 13:02
Operator : JC/MD
Sample : 02268-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50002-TOTE

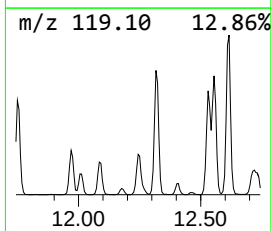
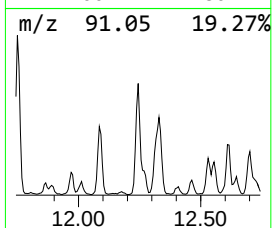
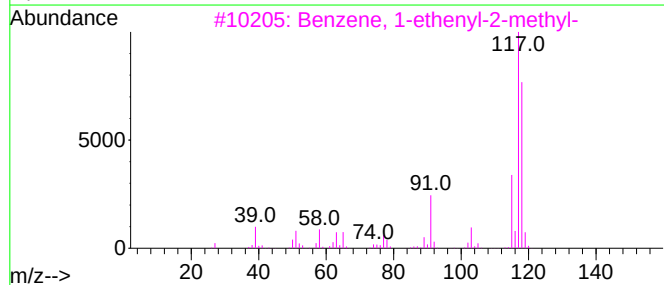
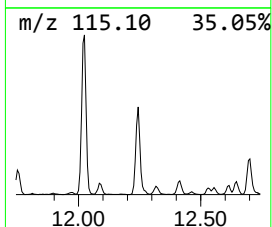
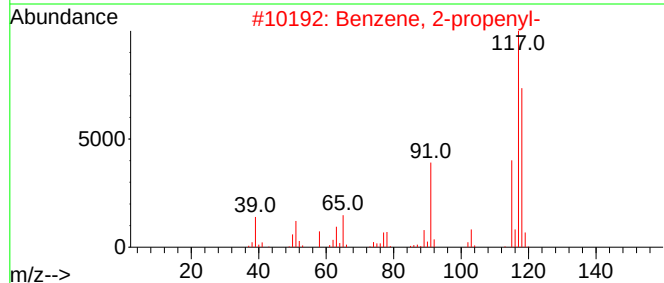
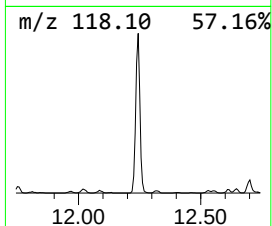
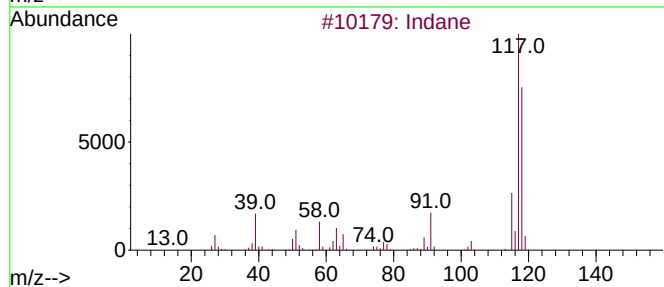
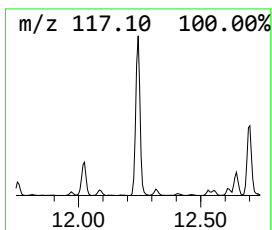
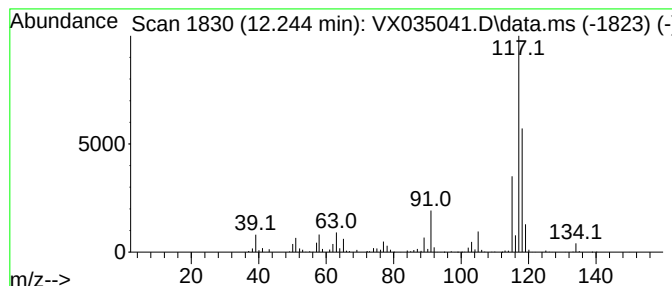
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Quant Title : SW846 8260

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

Peak Number 7 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	36.07 ug/l	780175	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	76
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	70
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	62
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041323\
Data File : VX035041.D
Acq On : 12 Apr 2023 13:02
Operator : JC/MD
Sample : 02268-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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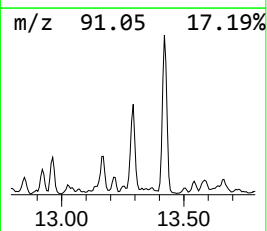
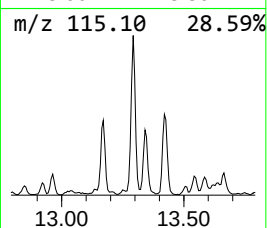
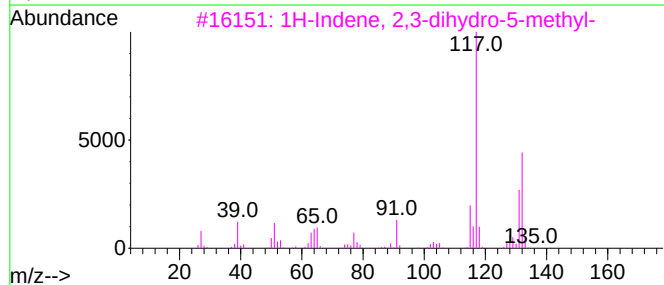
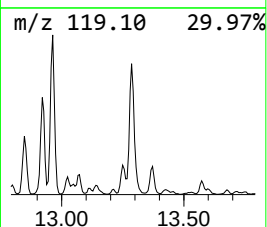
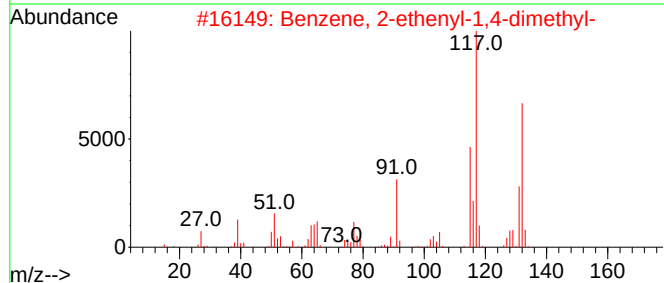
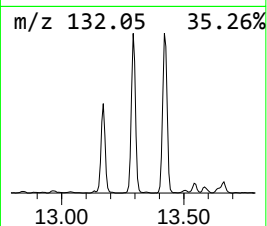
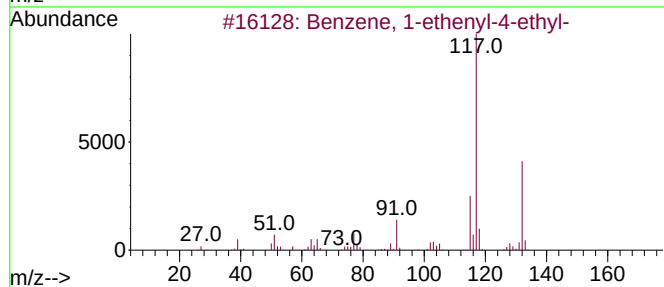
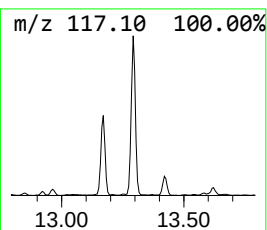
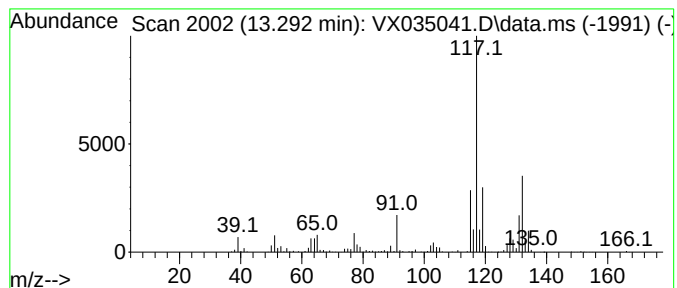
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	44.29 ug/l	957797	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			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041323\
Data File : VX035041.D
Acq On : 12 Apr 2023 13:02
Operator : JC/MD
Sample : 02268-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50002-TOTE

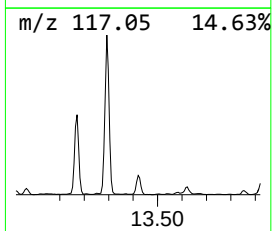
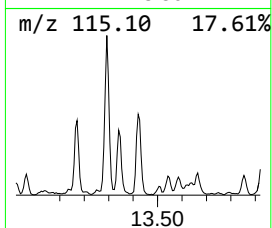
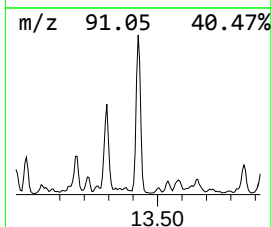
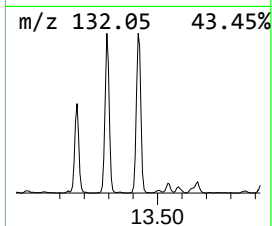
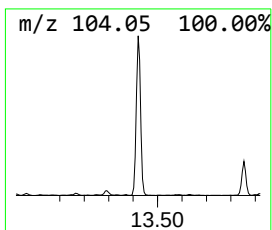
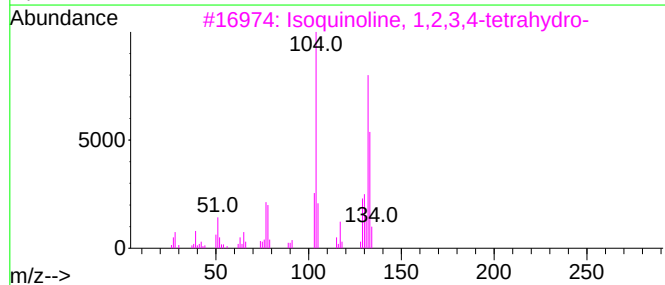
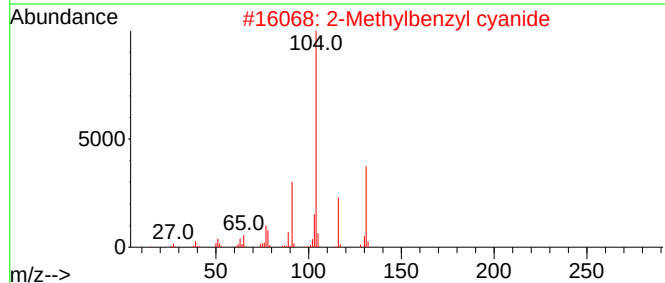
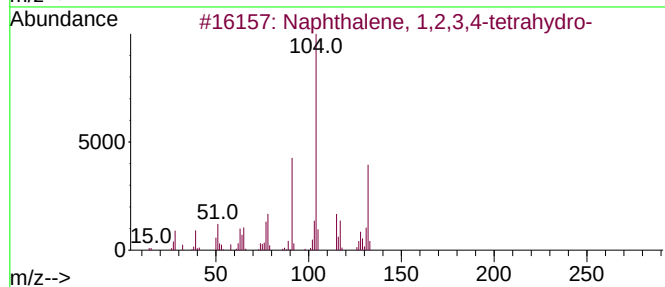
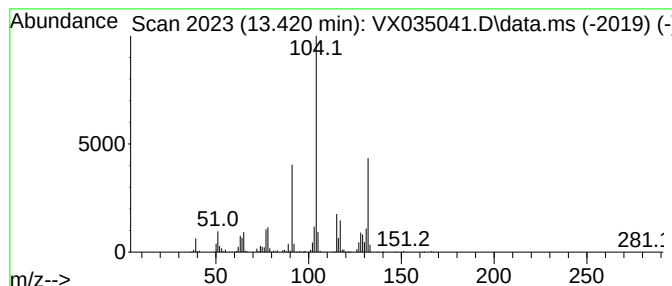
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	33.14 ug/l	716803	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	95
2			2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	43
3			Isoquinoline, 1,2,3,4-tetrahydro-	133	C9H11N	000091-21-4	43
4			Styrene	104	C8H8	000100-42-5	38
5			Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	007694-30-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041323\
Data File : VX035041.D
Acq On : 12 Apr 2023 13:02
Operator : JC/MD
Sample : 02268-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50002-TOTE

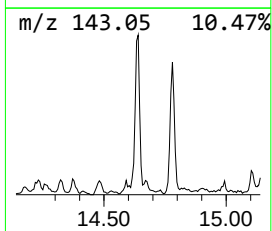
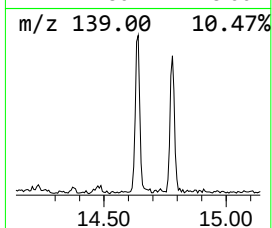
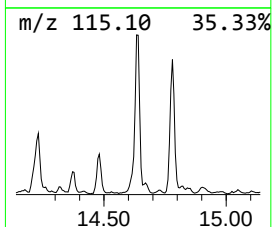
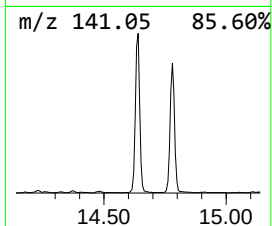
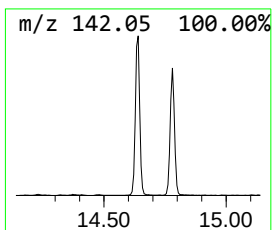
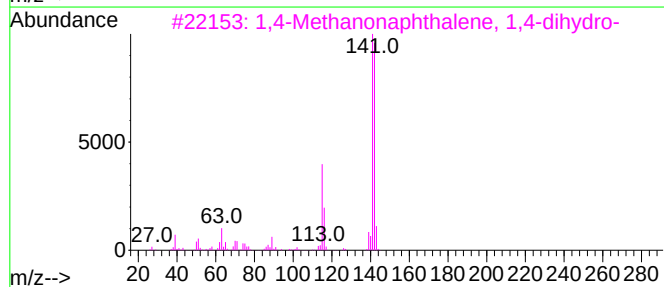
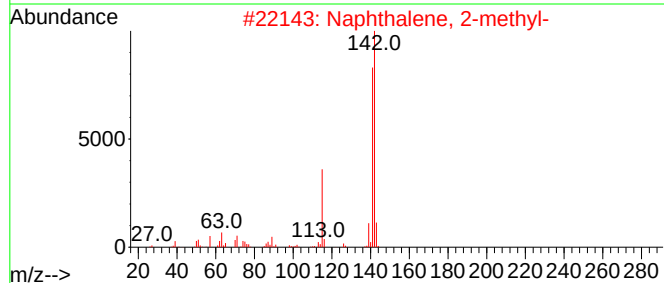
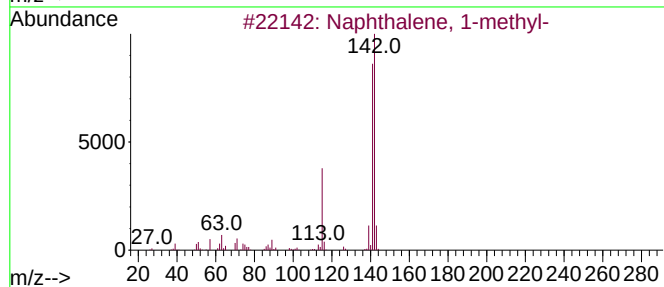
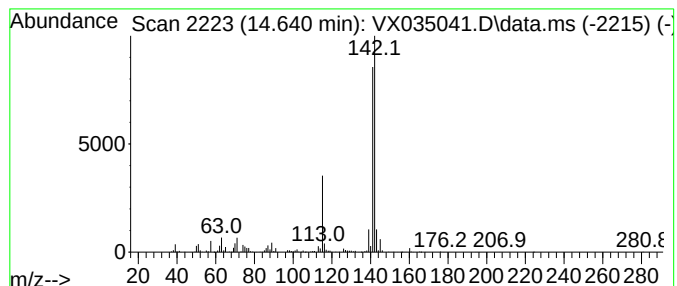
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Quant Title : SW846 8260

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

Peak Number 10 1,4-Methanonaphthalene, 1,4... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	28.39 ug/l	613901	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	90
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041323\
Data File : VX035041.D
Acq On : 12 Apr 2023 13:02
Operator : JC/MD
Sample : 02268-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50002-TOTE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.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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Ethanone, 1-oxi...	7.458	28.8	ug/l	620898	2	6.763	1078560	50.0
Benzene, 1-ethy...	11.378	38.1	ug/l	823636	4	12.024	1081370	50.0
Benzene, 1-ethy...	11.616	23.7	ug/l	512655	4	12.024	1081370	50.0
unknown11.969	11.969	25.6	ug/l	553075	4	12.024	1081370	50.0
Indane	12.244	36.1	ug/l	780175	4	12.024	1081370	50.0
Benzene, 2-ethe...	13.292	44.3	ug/l	957797	4	12.024	1081370	50.0
Naphthalene, 1,...	13.420	33.1	ug/l	716803	4	12.024	1081370	50.0
1,4-Methanonaph...	14.640	28.4	ug/l	613901	4	12.024	1081370	50.0