

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD110322\
 Data File : VD074720.D
 Acq On : 03 Nov 2022 17:27
 Operator : VA/SY
 Sample : N5204-01
 Misc : 5.02G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 20071

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_D\Method\82D110222S.M
 Title : SW846 8260

Signal : TIC: VD074720.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.728	18	24	35	rBV	596039	976470	56.00%	5.164%
2	2.417	136	141	150	rBV	24121	39784	2.28%	0.210%
3	3.899	383	393	401	rBV	8599	21109	1.21%	0.112%
4	4.017	401	413	434	rBV	544893	1495577	85.77%	7.909%
5	4.799	535	546	558	rVB2	45728	141706	8.13%	0.749%
6	5.040	573	587	589	rBV3	9528	26558	1.52%	0.140%
7	5.675	683	695	711	rBV2	26432	83844	4.81%	0.443%
8	5.840	713	723	734	rVB6	7359	22006	1.26%	0.116%
9	6.005	739	751	759	rBV4	9500	29579	1.70%	0.156%
10	6.805	875	887	899	rBV5	51597	168492	9.66%	0.891%
11	7.081	921	934	944	rBV3	83568	234886	13.47%	1.242%
12	7.805	1046	1057	1063	rBV	119540	287342	16.48%	1.520%
13	7.875	1063	1069	1080	rVB	122192	275991	15.83%	1.459%
14	8.228	1116	1129	1140	rVV	92015	218590	12.54%	1.156%
15	8.481	1164	1172	1179	rVB6	11584	27159	1.56%	0.144%
16	8.640	1190	1199	1207	rBV	188104	405189	23.24%	2.143%
17	8.775	1215	1222	1229	rBV	234452	473842	27.17%	2.506%
18	8.857	1229	1236	1248	rVB	199777	402864	23.10%	2.130%
19	9.222	1291	1298	1310	rVV	304248	568461	32.60%	3.006%
20	9.352	1313	1320	1331	rVB3	17193	41250	2.37%	0.218%
21	9.604	1355	1363	1375	rBV2	171670	372690	21.37%	1.971%
22	10.157	1451	1457	1467	rBV	97146	180795	10.37%	0.956%
23	10.269	1467	1476	1482	rBV	334757	608712	34.91%	3.219%
24	10.334	1482	1487	1491	rBV	111173	200199	11.48%	1.059%
25	10.440	1499	1505	1508	rBV2	13149	23333	1.34%	0.123%
26	10.481	1508	1512	1517	rVV2	14040	25480	1.46%	0.135%
27	10.540	1517	1522	1536	rVB3	13908	43329	2.48%	0.229%
28	10.775	1556	1562	1573	rVB	244566	466047	26.73%	2.465%
29	10.922	1578	1587	1593	rBV	80989	143819	8.25%	0.761%
30	11.022	1598	1604	1608	rBV2	31636	54108	3.10%	0.286%
31	11.069	1608	1612	1622	rVB	36384	67168	3.85%	0.355%
32	11.240	1630	1641	1647	rBV	132757	261170	14.98%	1.381%
33	11.298	1647	1651	1660	rVB2	45627	83894	4.81%	0.444%
34	11.422	1666	1672	1681	rBV2	46382	119703	6.86%	0.633%
35	11.546	1687	1693	1694	rBV2	32662	52597	3.02%	0.278%
36	11.581	1694	1699	1706	rVB	254767	432617	24.81%	2.288%

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Integrator: RTE

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37	11.669	1706	1714	1720	rBV2	169147	391077	22.43%	2.068%
38	11.716	1720	1722	1727	rVB3	42687	61111	3.50%	0.323%
39	11.787	1727	1734	1739	rBV	175326	355897	20.41%	1.882%
40	11.946	1755	1761	1768	rBV	100206	181403	10.40%	0.959%
41	12.022	1768	1774	1780	rVV	103334	183008	10.50%	0.968%
42	12.116	1783	1790	1798	rVV2	117310	201447	11.55%	1.065%
43	12.193	1798	1803	1808	rVB2	27151	42458	2.43%	0.225%
44	12.322	1816	1825	1835	rBV2	158786	320825	18.40%	1.697%
45	12.445	1835	1846	1849	rBV7	11542	30481	1.75%	0.161%
46	12.481	1849	1852	1855	rVV4	13082	23253	1.33%	0.123%
47	12.528	1855	1860	1862	rVV	99159	168857	9.68%	0.893%
48	12.569	1862	1867	1874	rVV2	235118	506187	29.03%	2.677%
49	12.640	1874	1879	1886	rVV2	95507	190186	10.91%	1.006%
50	12.716	1886	1892	1894	rVV2	33962	74230	4.26%	0.393%
51	12.769	1895	1901	1906	rVV3	74813	190430	10.92%	1.007%
52	12.822	1906	1910	1914	rVV3	100701	185790	10.66%	0.982%
53	12.893	1914	1922	1929	rVV3	183766	536641	30.78%	2.838%
54	13.063	1947	1951	1955	rVB	14685	20497	1.18%	0.108%
55	13.187	1966	1972	1979	rBV2	282087	529400	30.36%	2.800%
56	13.263	1980	1985	1991	rVB2	61633	126874	7.28%	0.671%
57	13.334	1991	1997	1999	rBV4	17805	32593	1.87%	0.172%
58	13.404	1999	2009	2019	rVV	976126	1743684	100.00%	9.221%
59	13.516	2020	2028	2038	rVV2	181741	491429	28.18%	2.599%
60	13.610	2038	2044	2050	rVB3	75521	158964	9.12%	0.841%
61	13.681	2050	2056	2059	rBV3	30406	63838	3.66%	0.338%
62	13.710	2059	2061	2062	rVV2	26041	25189	1.44%	0.133%
63	13.792	2065	2075	2083	rVV	302077	622208	35.68%	3.290%
64	13.869	2084	2088	2096	rVB3	53763	107999	6.19%	0.571%
65	13.957	2096	2103	2107	rBV6	16749	48291	2.77%	0.255%
66	14.010	2108	2112	2117	rVB7	13158	18450	1.06%	0.098%
67	14.069	2117	2122	2128	rBV3	36807	62751	3.60%	0.332%
68	14.222	2144	2148	2151	rBV4	15495	21249	1.22%	0.112%
69	14.257	2151	2154	2163	rVB8	24180	53373	3.06%	0.282%
70	14.340	2164	2168	2172	rBV4	15510	25049	1.44%	0.132%
71	14.387	2172	2176	2181	rVV	78421	121041	6.94%	0.640%
72	14.451	2181	2187	2190	rVV2	174081	315645	18.10%	1.669%
73	14.510	2194	2197	2200	rVV	96838	150408	8.63%	0.795%
74	14.551	2200	2204	2215	rVV3	118564	255885	14.67%	1.353%
75	14.645	2215	2220	2223	rVV	42138	70098	4.02%	0.371%
76	14.687	2223	2227	2232	rVV	61238	116009	6.65%	0.613%

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Title : SW846 8260

77	14.739	2232	2236	2248	rVB3	46812	85282	4.89%	0.451%
78	14.869	2253	2258	2264	rVB	148045	237713	13.63%	1.257%
79	14.934	2264	2269	2276	rVB4	20494	42774	2.45%	0.226%
80	15.028	2277	2285	2289	rBV	72748	146084	8.38%	0.773%
81	15.151	2300	2306	2312	rVB	67634	103972	5.96%	0.550%
82	15.216	2312	2317	2321	rBV3	22007	41466	2.38%	0.219%
83	15.275	2322	2327	2340	rVB5	48559	112883	6.47%	0.597%
84	15.434	2345	2354	2360	rBV10	10677	36156	2.07%	0.191%
85	15.592	2377	2381	2387	rVB2	21500	42820	2.46%	0.226%
86	15.816	2415	2419	2425	rVB7	15674	32474	1.86%	0.172%
87	15.963	2441	2444	2450	rVB7	12764	23892	1.37%	0.126%
88	16.069	2457	2462	2469	rBV7	13702	38133	2.19%	0.202%
89	16.139	2471	2474	2480	rVB5	9914	19393	1.11%	0.103%
90	16.381	2512	2515	2525	rVB3	21133	46643	2.67%	0.247%

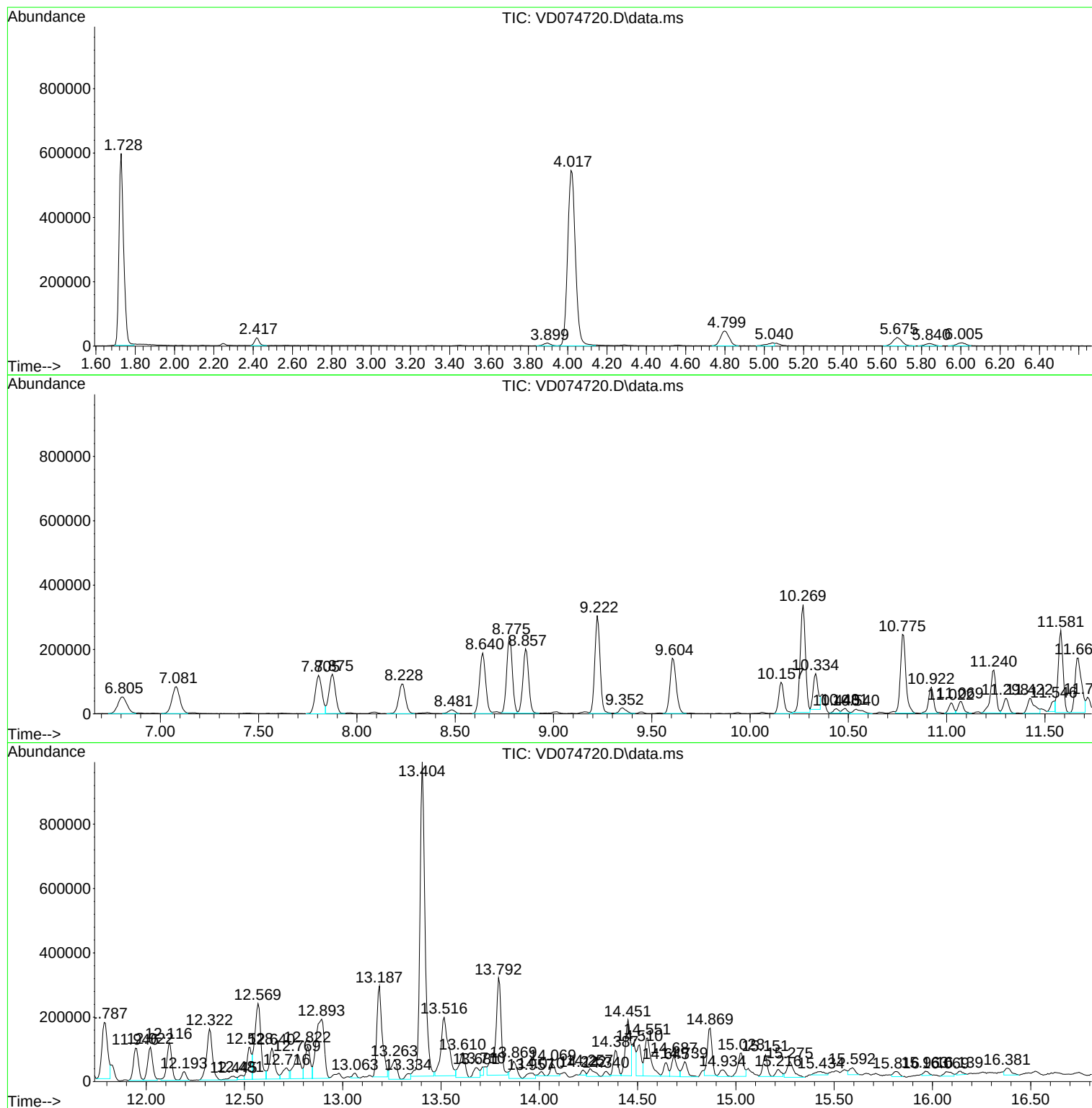
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Instrument :
MSVOA_D
ClientSampleId :
20071

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D110222S.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD110322\
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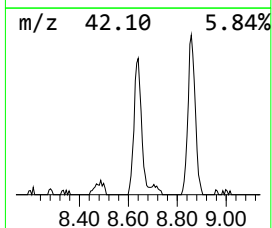
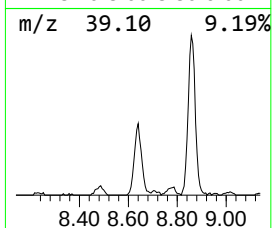
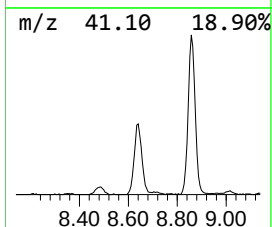
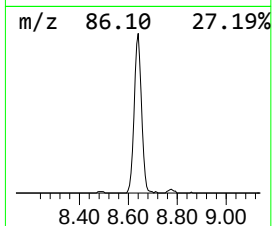
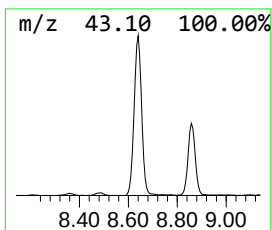
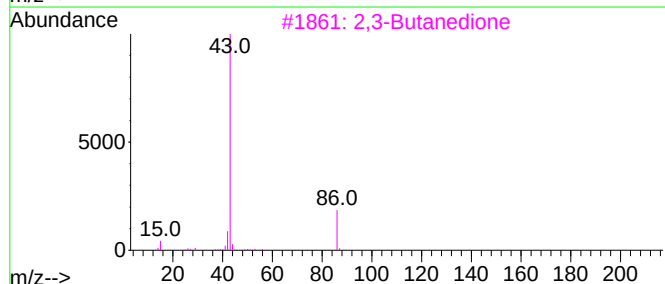
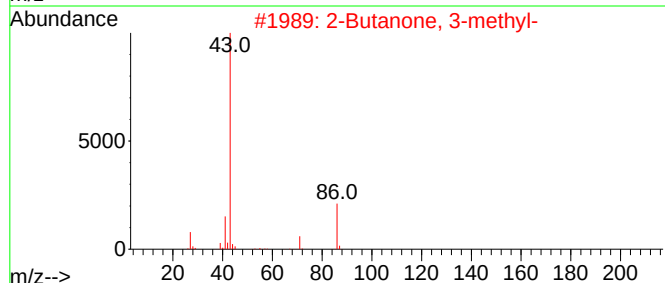
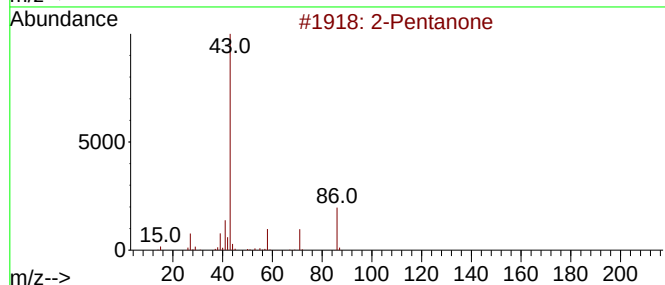
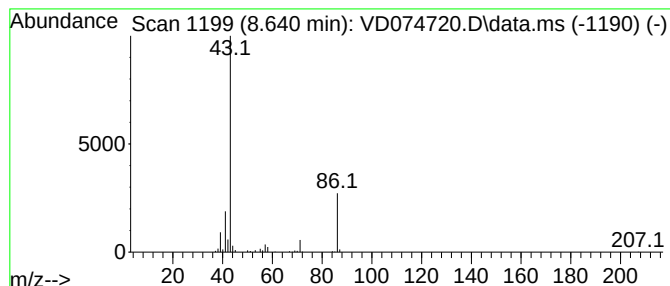
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D110222S.M
Quant Title : SW846 8260

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

Peak Number 2 2-Pentanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.640	42.76 ug/l	405189	1,4-Difluorobenzene	8.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone	86	C5H10O	000107-87-9	59
2			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	59
3			2,3-Butanedione	86	C4H6O2	000431-03-8	52
4			3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	45
5			Propanoic acid, 2-methyl-, 2-pro...	128	C7H12O2	015727-77-2	9



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Misc : 5.02G/5.00ml/MSVOA_D/SOIL
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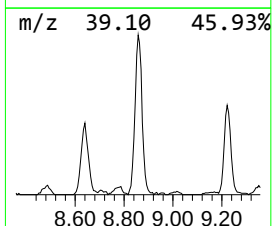
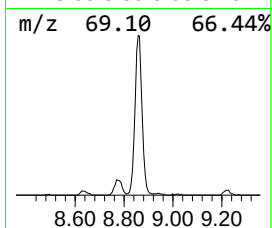
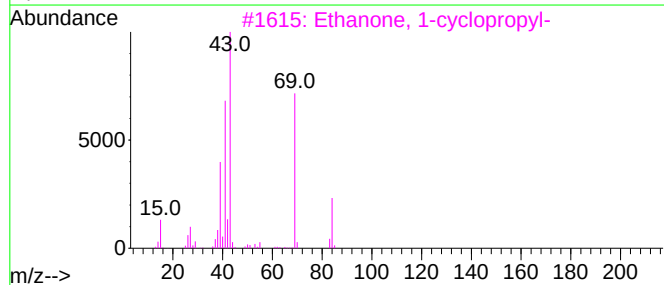
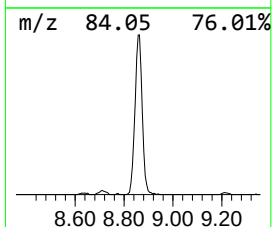
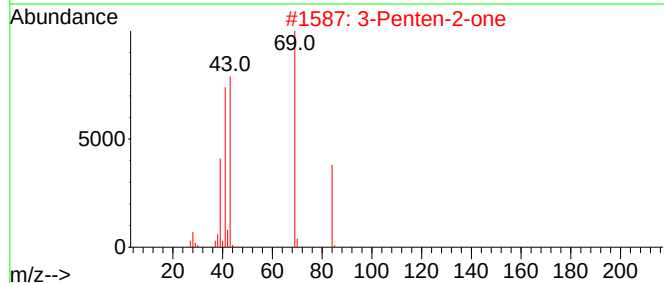
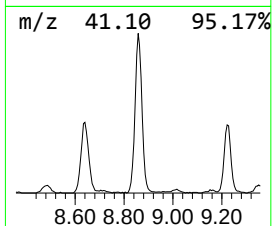
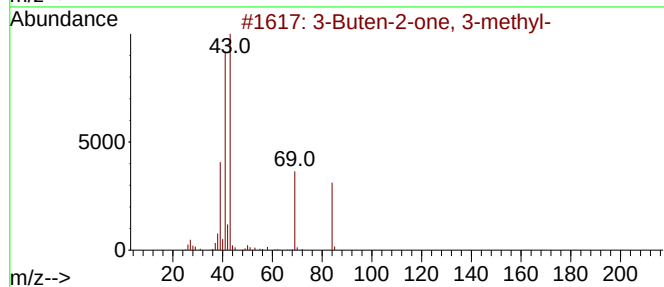
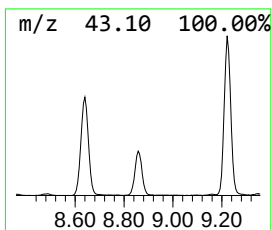
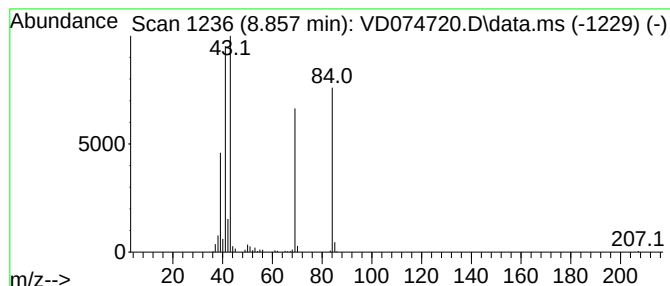
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D110222S.M
Quant Title : SW846 8260

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

Peak Number 3 3-Buten-2-one, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.857	42.51 ug/l	402864	1,4-Difluorobenzene	8.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	91
2			3-Penten-2-one	84	C5H8O	000625-33-2	78
3			Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	47
4			4H-1,2,4-Triazol-4-amine	84	C2H4N4	000584-13-4	43
5			2-Butanone, 4-hydroxy-3-(hydroxy...	132	C6H12O3	006868-97-9	40



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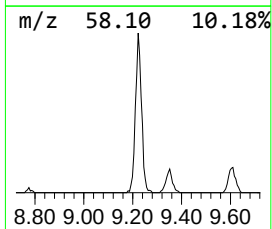
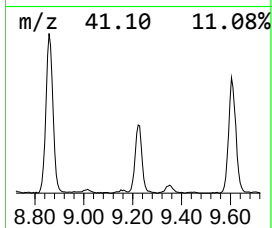
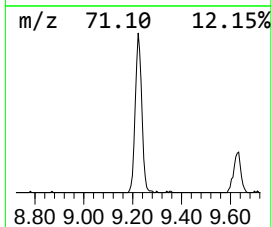
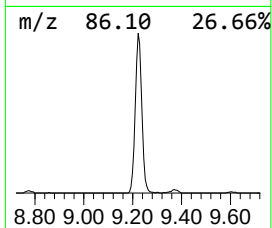
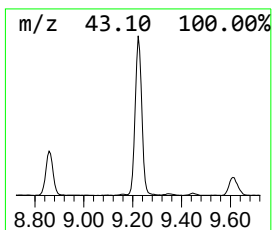
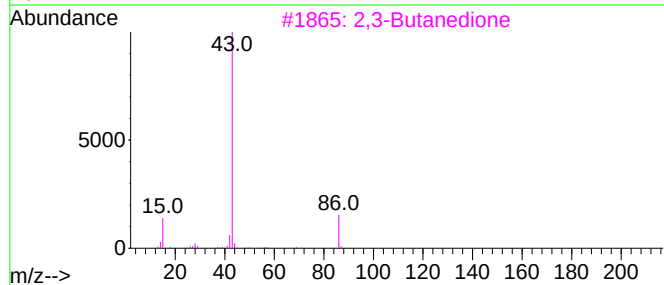
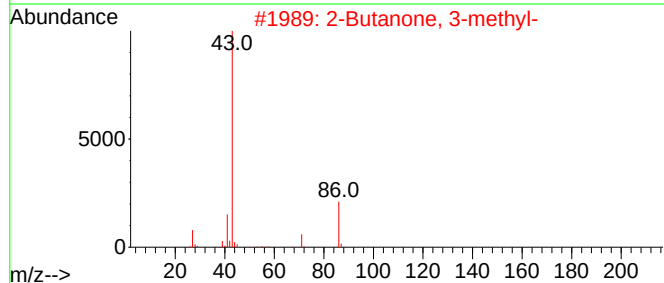
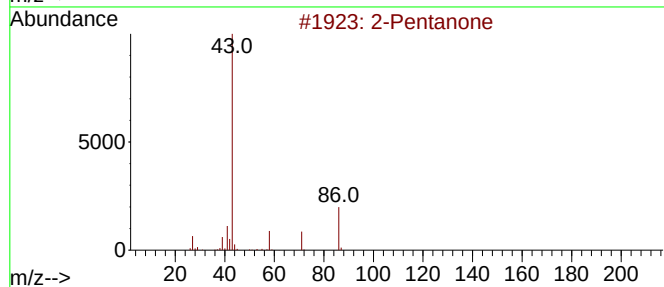
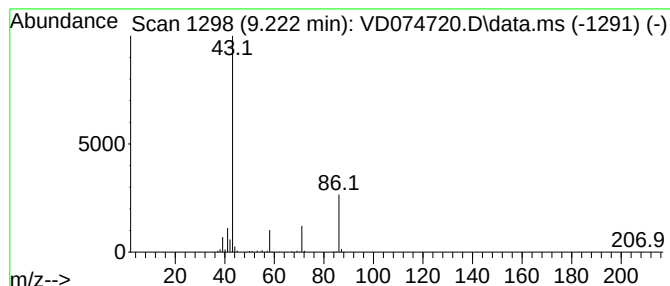
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D110222S.M
Quant Title : SW846 8260

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

Peak Number 4 2-Butanone, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.222	59.98 ug/l	568461	1,4-Difluorobenzene	8.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone	86	C5H10O	000107-87-9	87
2			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	53
3			2,3-Butanedione	86	C4H6O2	000431-03-8	52
4			Allyl acetate	100	C5H8O2	000591-87-7	17
5			3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	9



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ClientSampleId :
20071

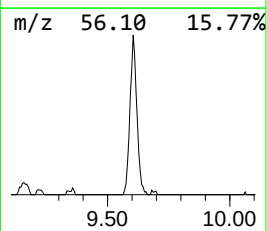
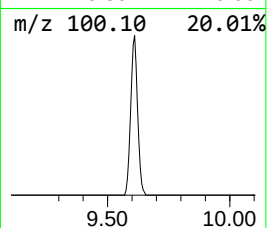
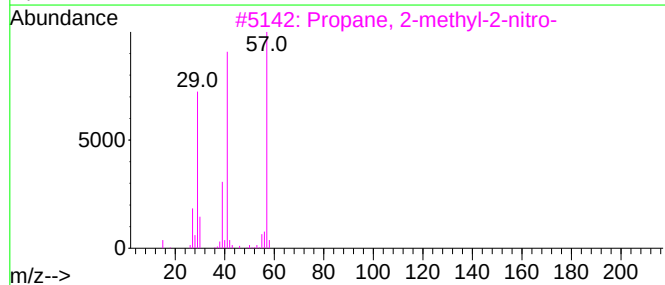
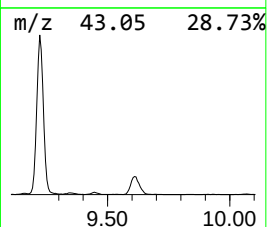
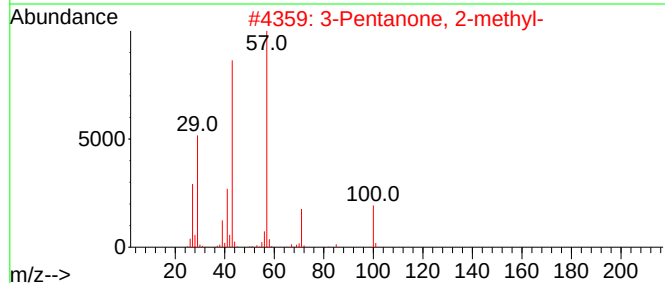
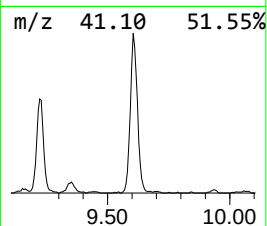
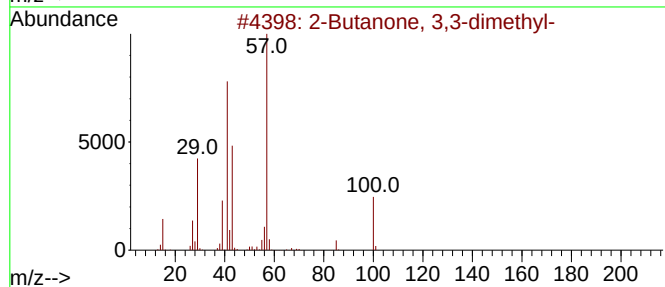
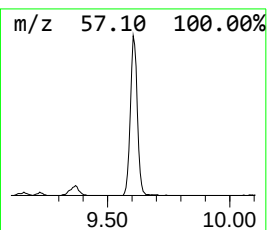
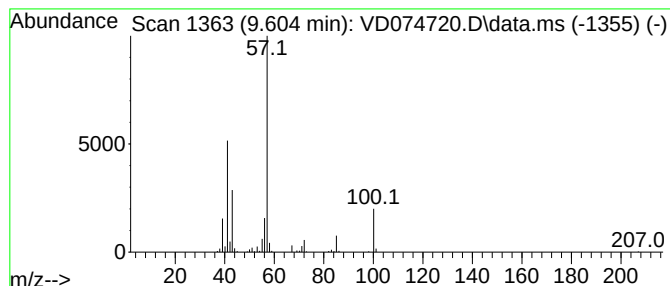
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Quant Title : SW846 8260

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

Peak Number 5 2-Butanone, 3,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.604	39.33 ug/l	372690	1,4-Difluorobenzene	8.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	86
2			3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	45
3			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	43
4			cis-1-Ethoxy-1-butene	100	C6H12O	1000139-43-8	42
5			Propane, 1-(ethenyloxy)-2-methyl-	100	C6H12O	000109-53-5	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD110322\
Data File : VD074720.D
Acq On : 03 Nov 2022 17:27
Operator : VA/SY
Sample : N5204-01
Misc : 5.02G/5.00ml/MSVOA_D/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
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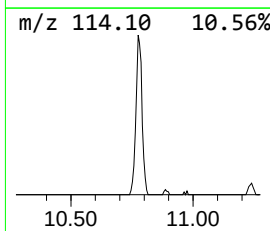
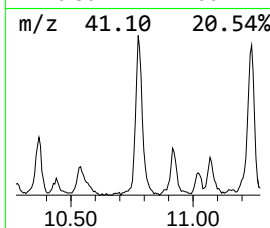
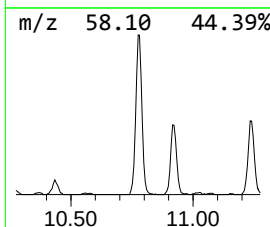
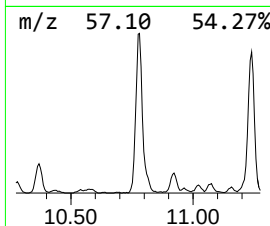
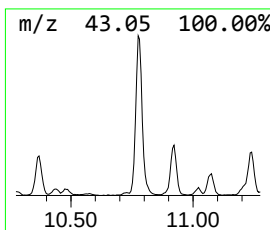
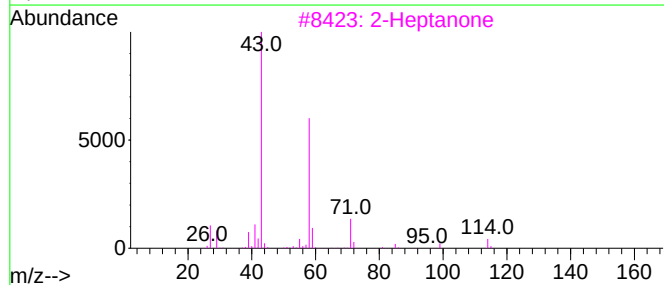
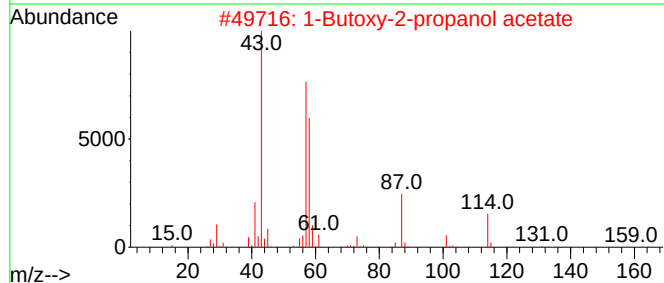
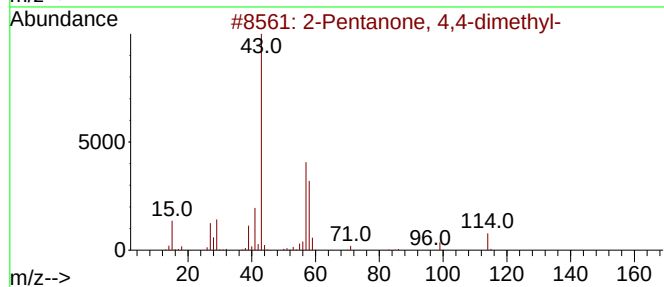
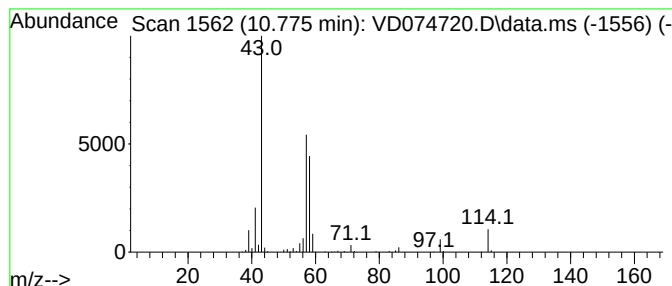
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Quant Title : SW846 8260

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

Peak Number 6 2-Pentanone, 4,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.775	53.86 ug/l	466047	Chlorobenzene-d5	11.581

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	91		
2	1-Butoxy-2-propanol acetate	174	C9H18O3	085409-76-3	64		
3	2-Heptanone	114	C7H14O	000110-43-0	42		
4	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	39		
5	1-Butoxypropan-2-yl 2-methylbuta...	216	C12H24O3	1000367-09-4	35		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD110322\
Data File : VD074720.D
Acq On : 03 Nov 2022 17:27
Operator : VA/SY
Sample : N5204-01
Misc : 5.02G/5.00ml/MSVOA_D/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
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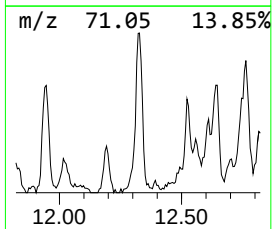
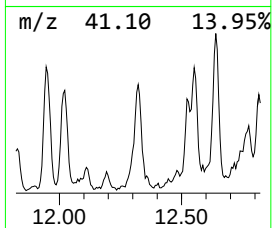
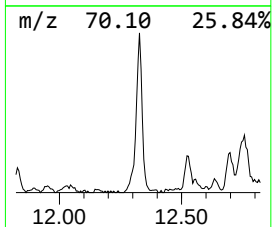
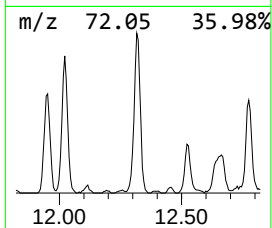
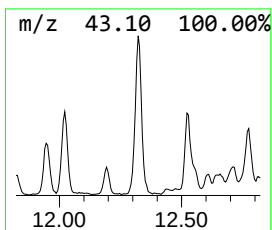
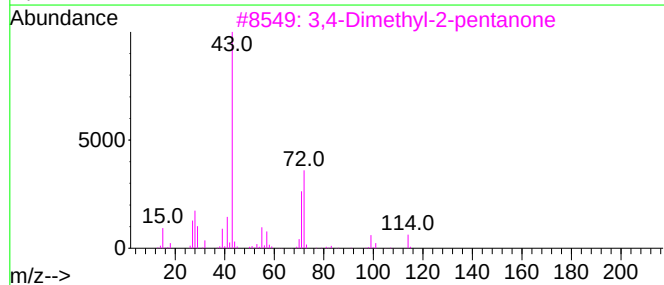
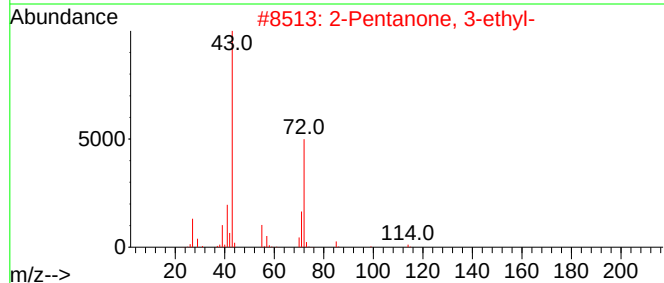
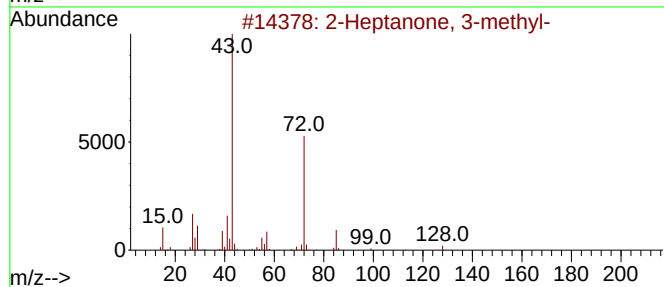
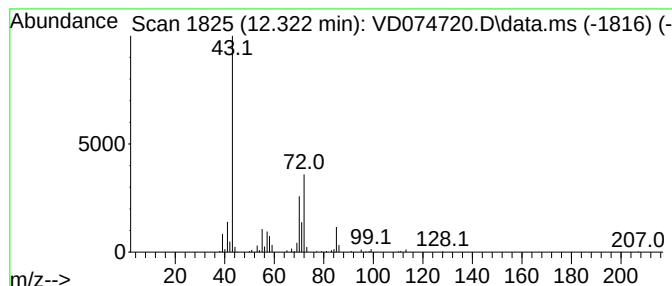
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Quant Title : SW846 8260

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

Peak Number 7 unknown12.322 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.322	37.08 ug/l	320825	Chlorobenzene-d5	11.581

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone, 3-methyl-	128	C8H16O	002371-19-9	47
2			2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	47
3			3,4-Dimethyl-2-pentanone	114	C7H14O	1000202-23-1	43
4			2-Hexanone, 3-methyl-	114	C7H14O	002550-21-2	40
5			trans-2,3-Epoxydecane	156	C10H20O	054125-39-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD110322\
Data File : VD074720.D
Acq On : 03 Nov 2022 17:27
Operator : VA/SY
Sample : N5204-01
Misc : 5.02G/5.00ml/MSVOA_D/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
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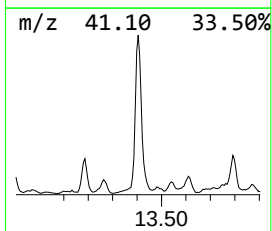
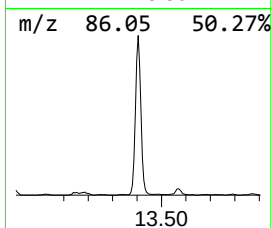
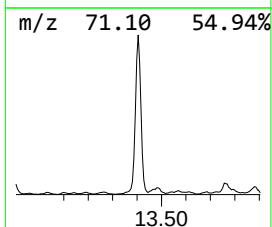
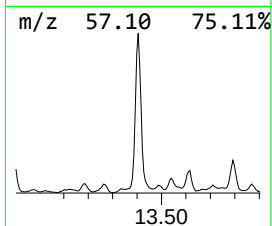
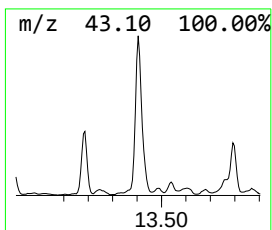
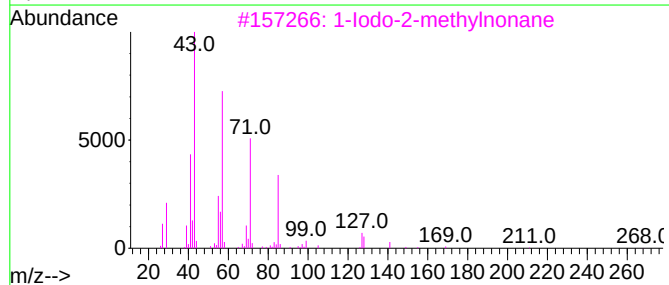
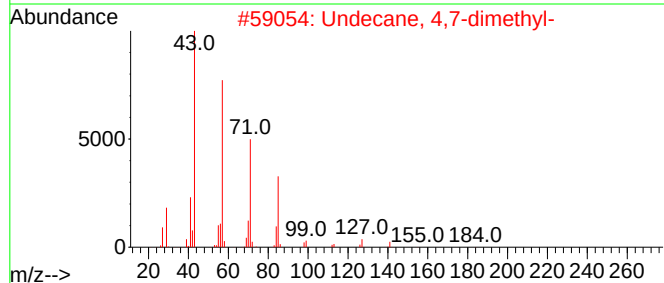
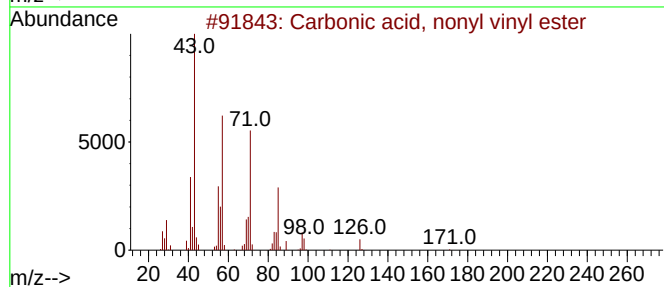
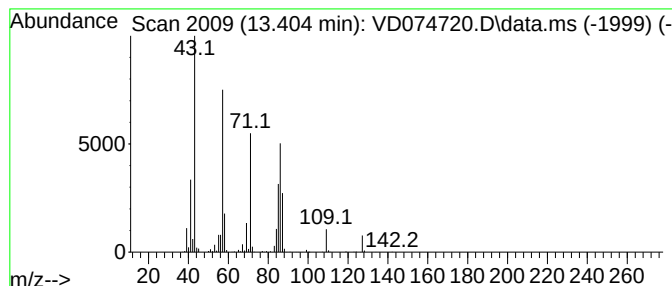
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Quant Title : SW846 8260

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

Peak Number 8 unknown13.404 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.404	177.41 ug/l	1743680	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	43
2			Undecane, 4,7-dimethyl-	184	C13H28	017301-32-5	38
3			1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	37
4			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	35
5			Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD110322\
Data File : VD074720.D
Acq On : 03 Nov 2022 17:27
Operator : VA/SY
Sample : N5204-01
Misc : 5.02G/5.00ml/MSVOA_D/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
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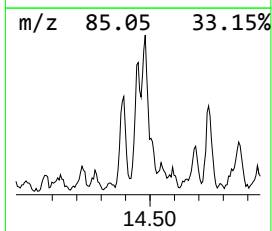
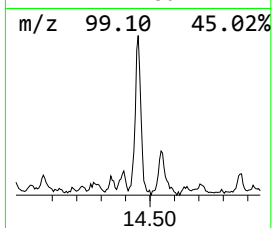
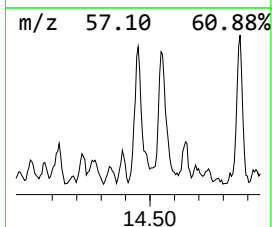
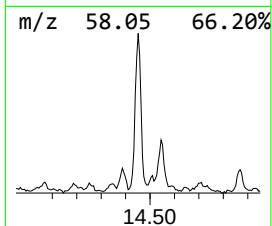
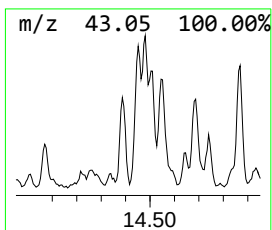
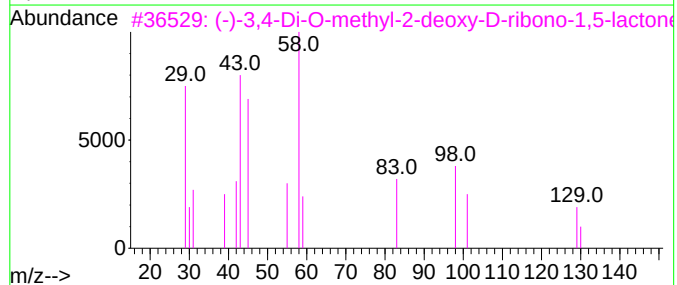
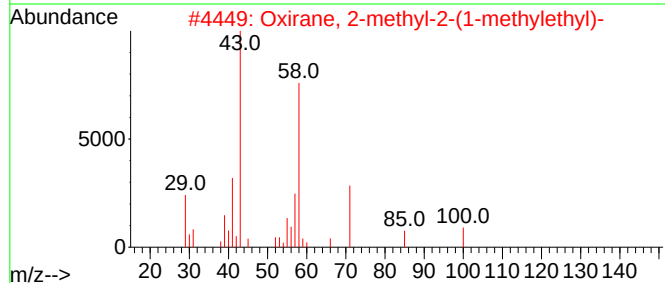
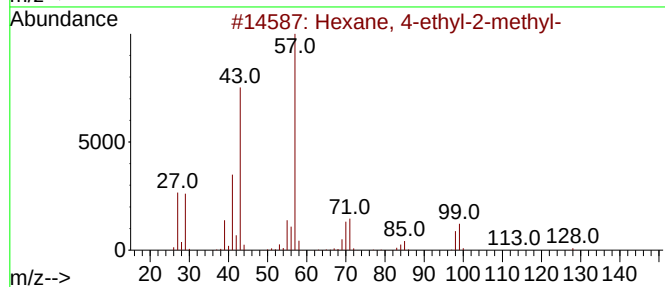
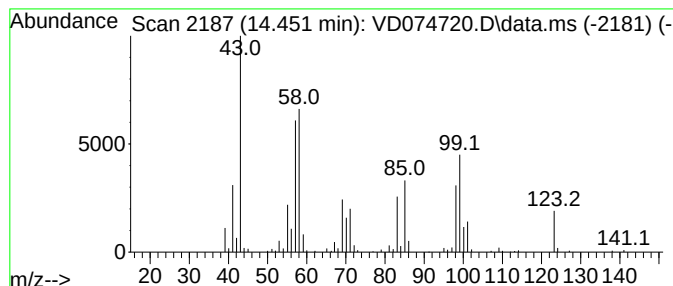
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Quant Title : SW846 8260

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

Peak Number 10 unknown14.451 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.451	32.12 ug/l	315645	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 4-ethyl-2-methyl-	128	C9H20	003074-75-7	25
2			Oxirane, 2-methyl-2-(1-methyleth...	100	C6H12O	072221-03-5	22
3			(-)-3,4-Di-O-methyl-2-deoxy-D-ri...	160	C7H12O4	085921-57-9	16
4			2-Methoxyethyl 2-methylbutanoate	160	C8H16O3	1000366-96-4	14
5			Hexanoic acid, 2-propenyl ester	156	C9H16O2	000123-68-2	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD110322\
Data File : VD074720.D
Acq On : 03 Nov 2022 17:27
Operator : VA/SY
Sample : N5204-01
Misc : 5.02G/5.00ml/MSVOA_D/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
20071

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D110222S.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
2-Pentanone	8.640	42.8	ug/l	405189	2	8.775	473842	50.0
3-Buten-2-one, ...	8.857	42.5	ug/l	402864	2	8.775	473842	50.0
2-Butanone, 3-m...	9.222	60.0	ug/l	568461	2	8.775	473842	50.0
2-Butanone, 3,3...	9.604	39.3	ug/l	372690	2	8.775	473842	50.0
2-Pentanone, 4...	10.775	53.9	ug/l	466047	3	11.581	432617	50.0
unknown12.322	12.322	37.1	ug/l	320825	3	11.581	432617	50.0
unknown13.404	13.404	177.4	ug/l	1743680	4	13.516	491429	50.0
unknown14.451	14.451	32.1	ug/l	315645	4	13.516	491429	50.0