

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD062223\
 Data File : VD076547.D
 Acq On : 22 Jun 2023 19:12
 Operator : KP/SY
 Sample : 03365-24
 Misc : 5.00G/5.0ml/MSVOA_D/SOIL
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 TP1

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\82D061623S.M
 Title : SW846 8260

Signal : TIC: VD076547.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.734	19	25	34	rBV	114723	212532	100.00%	16.286%
2	1.887	47	51	55	rVB2	2269	3214	1.51%	0.246%
3	2.158	90	97	99	rBV2	2646	4168	1.96%	0.319%
4	2.181	99	101	103	rVV	2264	2598	1.22%	0.199%
5	2.240	110	111	117	rVB4	2169	3017	1.42%	0.231%
6	2.875	218	219	224	rVB2	3043	3522	1.66%	0.270%
7	2.993	236	239	240	rBV2	2514	2276	1.07%	0.174%
8	4.811	546	548	554	rVB2	1711	2504	1.18%	0.192%
9	7.063	923	931	932	rBV2	6304	9151	4.31%	0.701%
10	7.805	1047	1057	1063	rBV2	13844	32873	15.47%	2.519%
11	7.875	1063	1069	1075	rVB2	17002	34351	16.16%	2.632%
12	8.228	1124	1129	1136	rVB2	17685	36190	17.03%	2.773%
13	8.775	1212	1222	1228	rBV	29871	60495	28.46%	4.636%
14	9.352	1319	1320	1325	rBV2	1669	2216	1.04%	0.170%
15	9.940	1417	1420	1423	rBV2	1885	2523	1.19%	0.193%
16	10.269	1469	1476	1486	rVB	46830	81504	38.35%	6.245%
17	10.410	1498	1500	1504	rBV3	2242	2147	1.01%	0.165%
18	10.528	1519	1520	1525	rBV4	1658	2341	1.10%	0.179%
19	10.816	1566	1569	1574	rBV3	1954	2859	1.35%	0.219%
20	11.034	1601	1606	1607	rBV4	2844	4529	2.13%	0.347%
21	11.193	1628	1633	1635	rVB4	2124	2511	1.18%	0.192%
22	11.269	1643	1646	1648	rVV2	2727	3069	1.44%	0.235%
23	11.340	1655	1658	1661	rBV5	2301	2852	1.34%	0.219%
24	11.387	1664	1666	1669	rVV3	2513	2706	1.27%	0.207%
25	11.428	1669	1673	1677	rVB5	1884	3399	1.60%	0.260%
26	11.581	1692	1699	1706	rBV	50275	90023	42.36%	6.898%
27	11.957	1761	1763	1766	rVB4	3134	2273	1.07%	0.174%
28	11.993	1766	1769	1770	rBV2	2656	2549	1.20%	0.195%
29	12.257	1813	1814	1816	rBV2	3107	2200	1.04%	0.169%
30	12.369	1829	1833	1834	rBV4	6366	7260	3.42%	0.556%
31	12.428	1837	1843	1844	rBV6	7179	11139	5.24%	0.854%
32	12.451	1845	1847	1850	rVV4	4201	5434	2.56%	0.416%
33	12.575	1862	1868	1874	rVB3	38805	71358	33.58%	5.468%
34	12.622	1874	1876	1880	rBV4	1971	3224	1.52%	0.247%
35	12.693	1885	1888	1889	rBV3	4685	4736	2.23%	0.363%
36	12.781	1899	1903	1906	rBV6	6377	8922	4.20%	0.684%

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

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37	12.881	1918	1920	1921	rBV3	3455	2239	1.05%	0.172%
38	13.075	1951	1953	1956	rBV4	4070	3799	1.79%	0.291%
39	13.263	1983	1985	1986	rBV2	2920	2215	1.04%	0.170%
40	13.293	1988	1990	1991	rBV2	3276	2477	1.17%	0.190%
41	13.322	1992	1995	1997	rBV4	4714	5101	2.40%	0.391%
42	13.357	1997	2001	2002	rBV4	5333	5672	2.67%	0.435%
43	13.387	2004	2006	2007	rBV2	8401	6579	3.10%	0.504%
44	13.516	2023	2028	2035	rVB	61813	103618	48.75%	7.940%
45	13.640	2040	2049	2061	rVB8	44147	158905	74.77%	12.177%
46	13.763	2068	2070	2071	rBV2	4223	2529	1.19%	0.194%
47	13.828	2075	2081	2086	rVV10	13812	36402	17.13%	2.789%
48	14.169	2135	2139	2140	rBV4	11280	11651	5.48%	0.893%
49	14.445	2184	2186	2190	rBV5	4974	8430	3.97%	0.646%
50	15.016	2281	2283	2284	rBV2	6640	4557	2.14%	0.349%
51	15.110	2297	2299	2302	rBV4	7574	8279	3.90%	0.634%
52	15.369	2335	2343	2353	rVB4	21964	67669	31.84%	5.185%
53	15.487	2360	2363	2370	rBV9	7375	17033	8.01%	1.305%
54	15.645	2382	2390	2400	rVB9	28140	97462	45.86%	7.468%
55	16.081	2462	2464	2467	rBV4	4219	4329	2.04%	0.332%
56	16.234	2486	2490	2491	rBV4	5448	7683	3.61%	0.589%
57	16.269	2494	2496	2501	rVB6	7403	10108	4.76%	0.775%
58	16.704	2569	2570	2572	rBV2	3021	2195	1.03%	0.168%
59	16.734	2572	2575	2576	rVV3	5166	4387	2.06%	0.336%
60	16.757	2576	2579	2581	rVB4	2599	3026	1.42%	0.232%

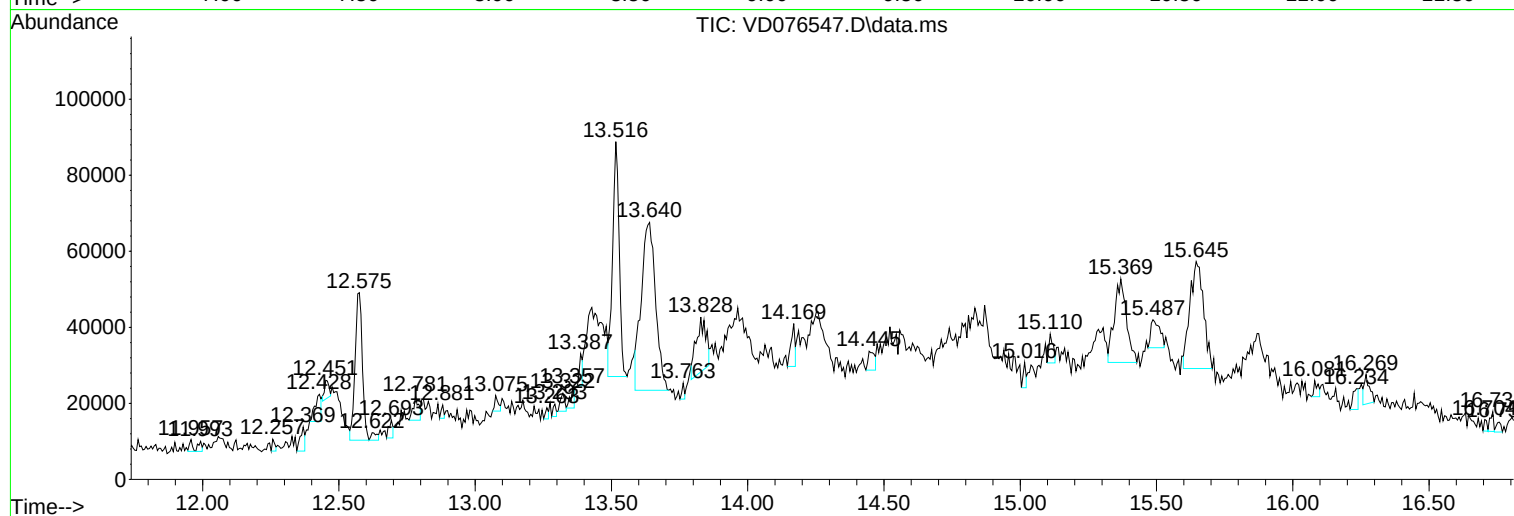
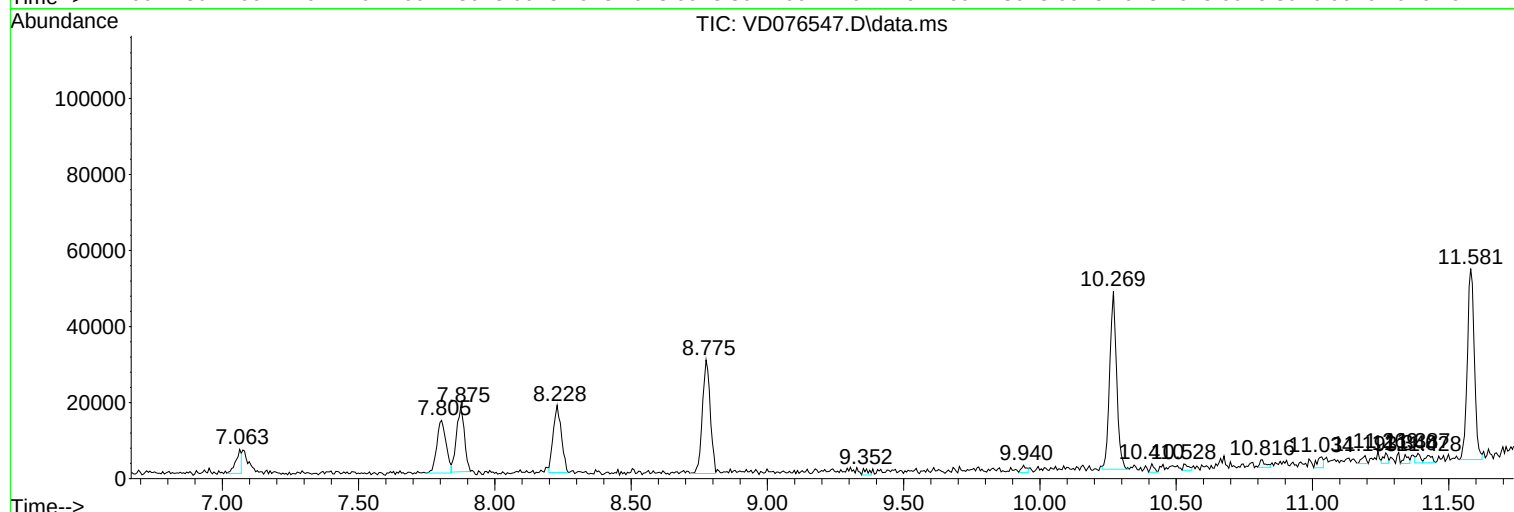
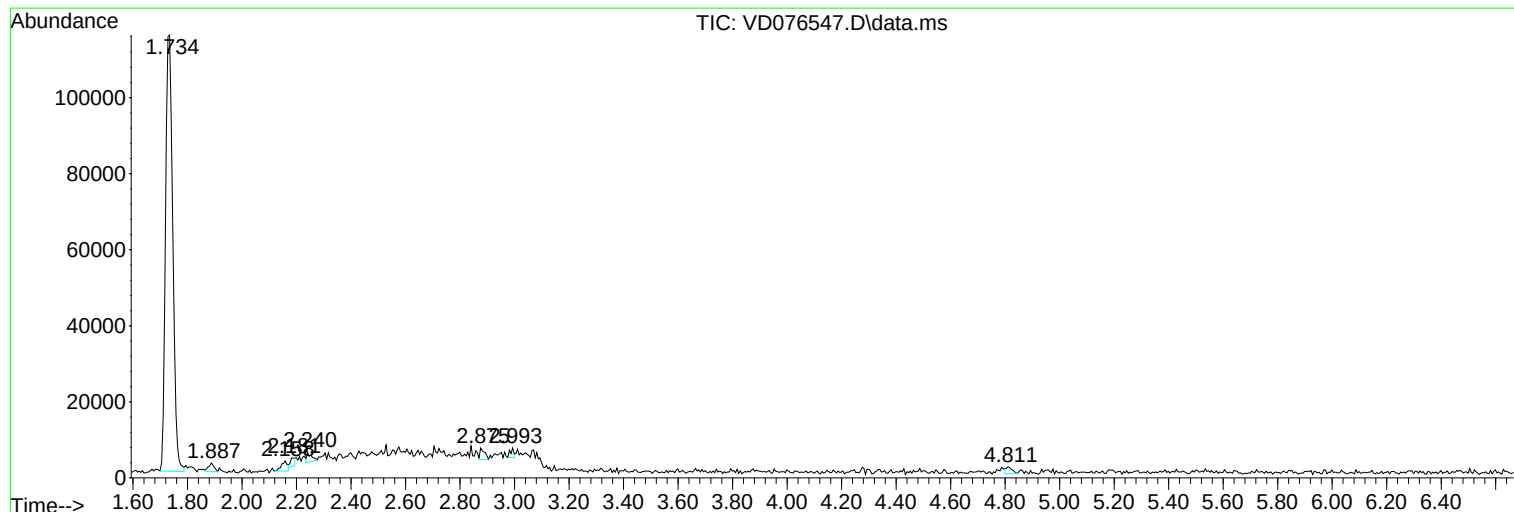
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D061623S.M
Quant Title : SW846 8260

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



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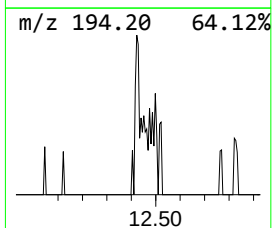
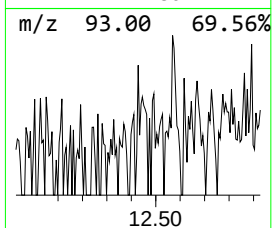
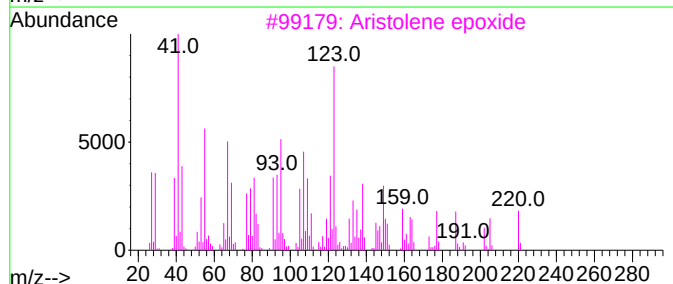
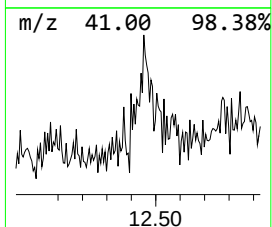
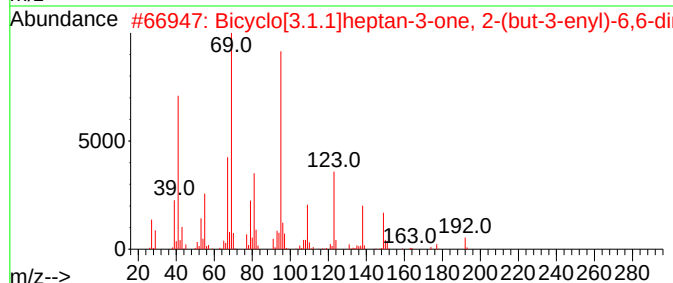
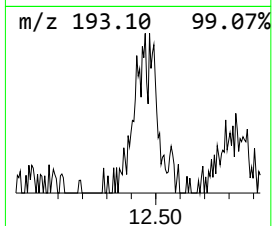
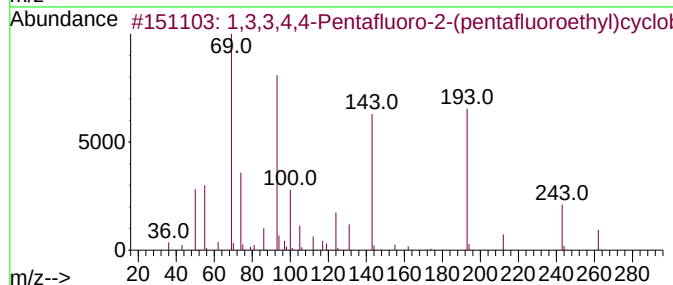
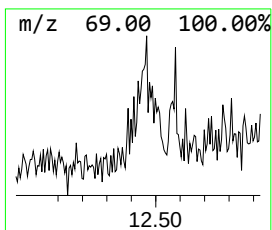
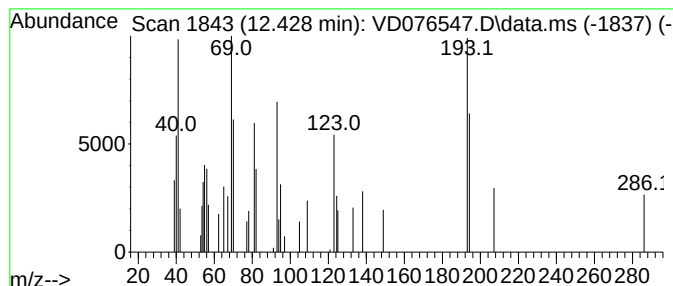
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D061623S.M
Quant Title : SW846 8260

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

Peak Number 4 unknown12.428 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.428	6.19 ug/l	11139	Chlorobenzene-d5	11.581

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,3,4,4-Pentafluoro-2-(pentafl...	262	C6F10	1000394-46-8	16
2			Bicyclo[3.1.1]heptan-3-one, 2-(b...	192	C13H20O	1010163-96-1	12
3			Aristolene epoxide	220	C15H24O	1000151-48-9	10
4			7-Nitro-2,4-dihydro-1,4-benzoxaz...	194	C8H6N2O4	081721-86-0	10
5			2-Butenoic acid, 3,7-dimethyl-6-...	224	C14H24O2	068039-38-3	10



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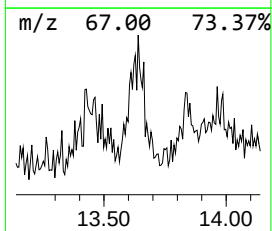
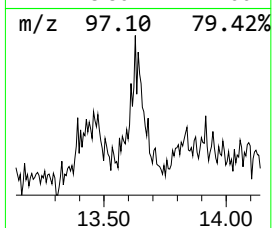
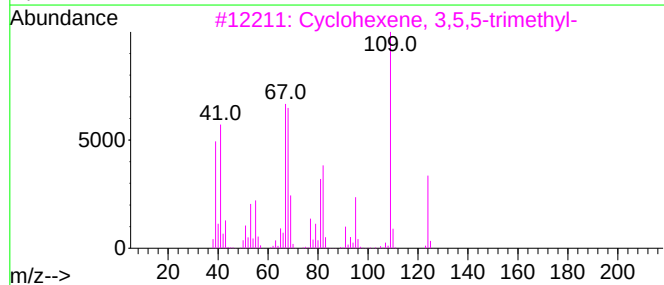
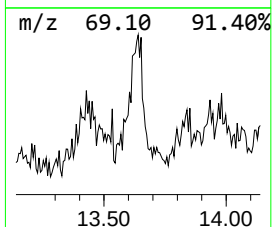
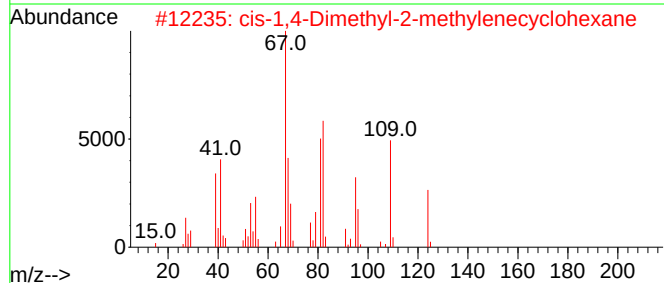
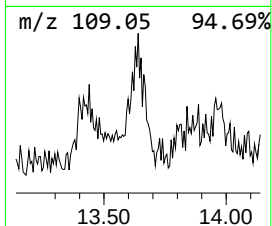
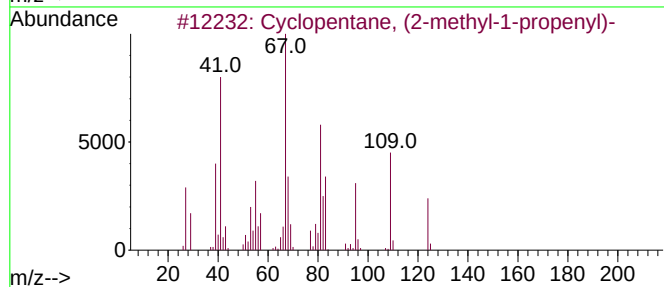
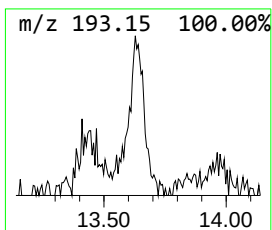
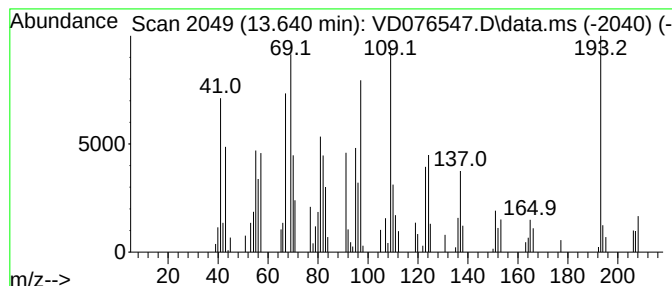
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D061623S.M
Quant Title : SW846 8260

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

Peak Number 5 unknown13.640 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.640	76.68 ug/l	158905	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, (2-methyl-1-propen...	124	C9H16	053366-57-7	35
2			cis-1,4-Dimethyl-2-methylenecycl...	124	C9H16	019781-46-5	35
3			Cyclohexene, 3,5,5-trimethyl-	124	C9H16	000933-12-0	30
4			Cyclopropane, 1,1-dimethyl-2-(2...	124	C9H16	033422-32-1	30
5			Hexane, 1-(isopropylidenecyclopr...	166	C12H22	024524-53-6	27



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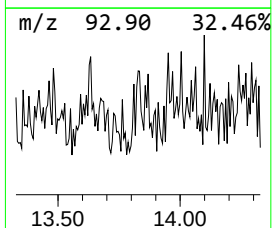
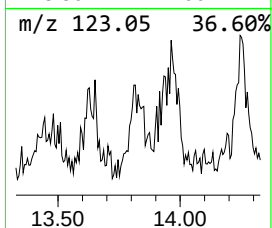
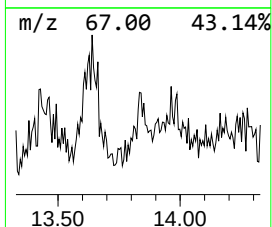
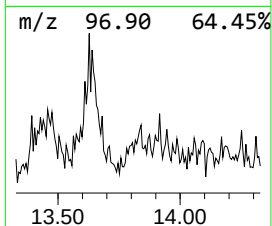
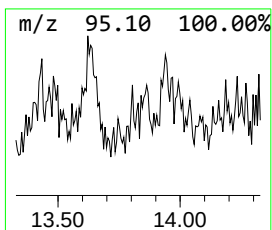
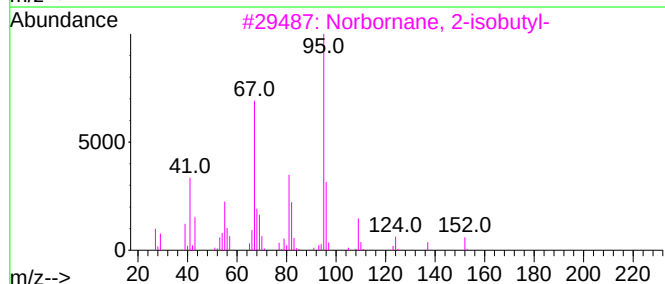
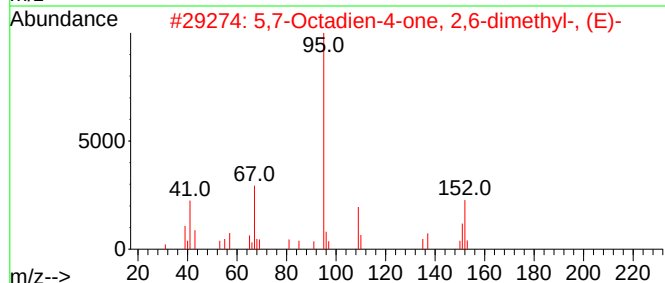
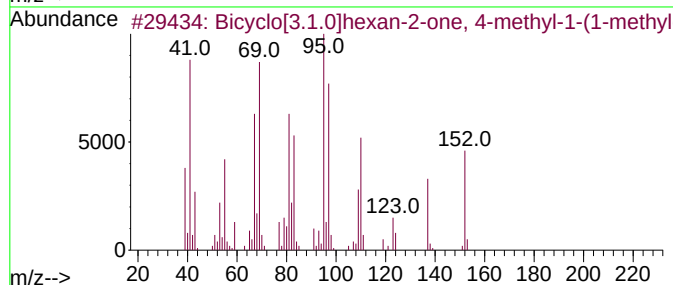
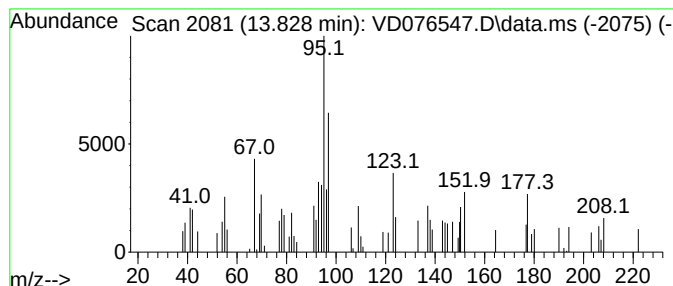
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Quant Title : SW846 8260

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

Peak Number 6 unknown13.828 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.828	17.57 ug/l	36402	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.1.0]hexan-2-one, 4-met...	152	C10H16O	002506-61-8	47
2			5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	38
3			Norbornane, 2-isobutyl-	152	C11H20	018127-14-5	38
4			3-t-Butyl-6-methyl-2H-pyran	152	C10H16O	1000188-12-8	38
5			Diisopropylaminoacrylonitril	152	C9H16N2	038691-28-0	35



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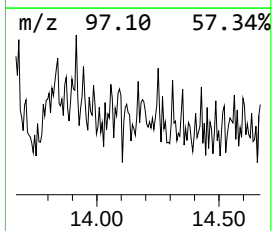
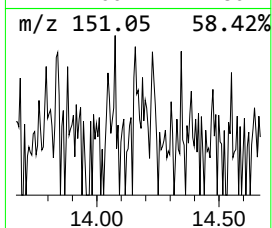
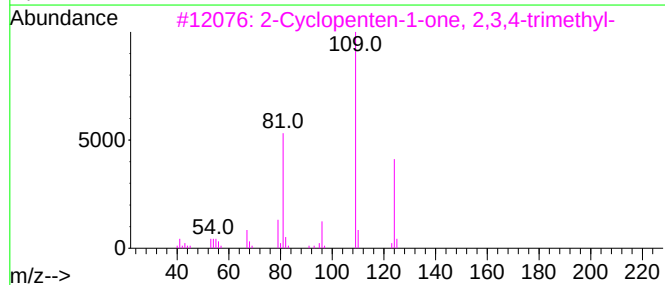
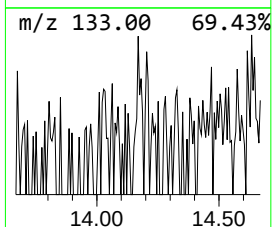
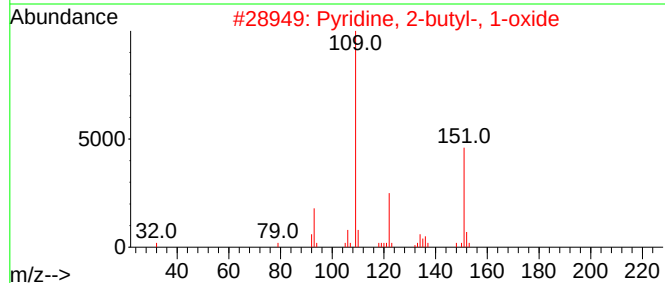
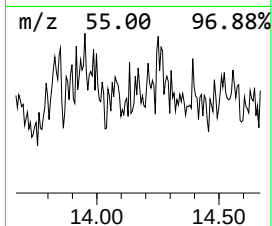
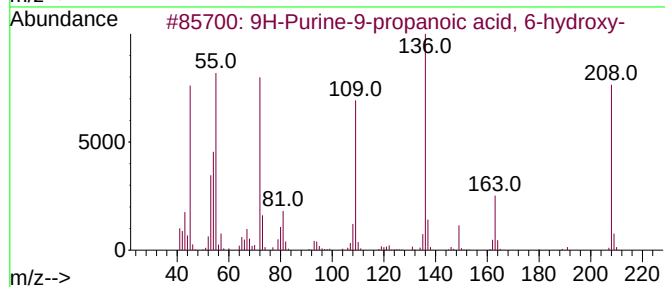
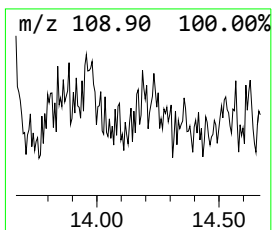
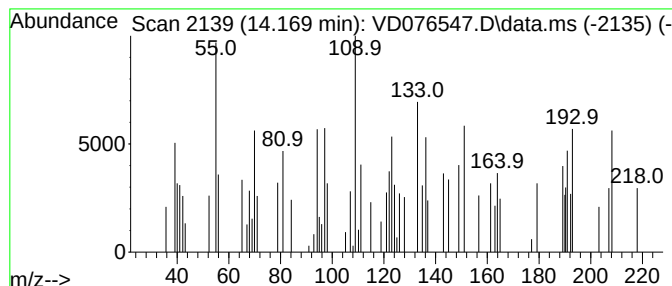
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D061623S.M
Quant Title : SW846 8260

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

Peak Number 7 unknown14.169 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.169	5.62 ug/l	11651	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Purine-9-propanoic acid, 6-hy...	208	C8H8N4O3	034397-00-7	25		
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	18		
3	2-Cyclopenten-1-one, 2,3,4-trime...	124	C8H12O	028790-86-5	11		
4	Benzene, 2,4-dichloro-1-nitro-	191	C6H3Cl2NO2	000611-06-3	11		
5	1,1-Dimethyl-1-silacyclo-2,4-hex...	124	C7H12Si	052023-18-4	11		



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Sample : 03365-24
Misc : 5.00G/5.0ml/MSVOA_D/SOIL
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
TP1

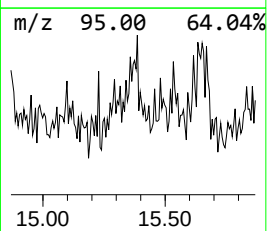
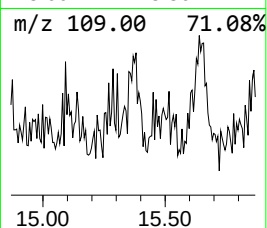
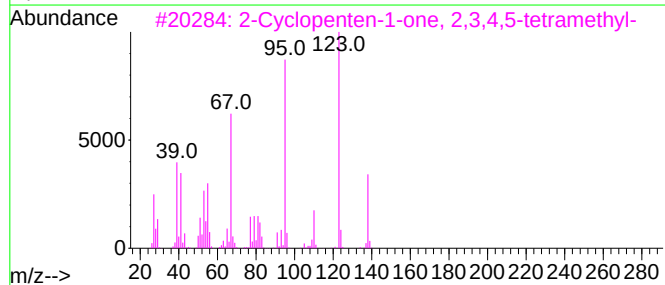
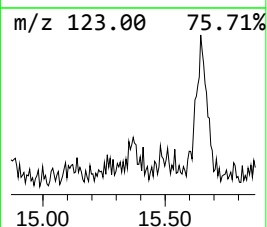
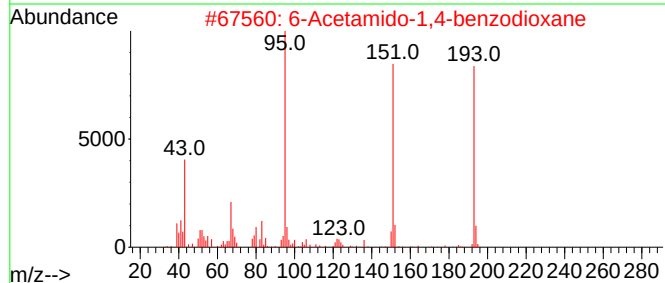
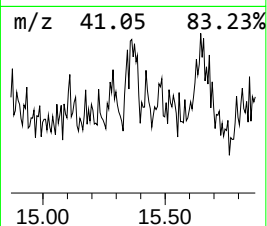
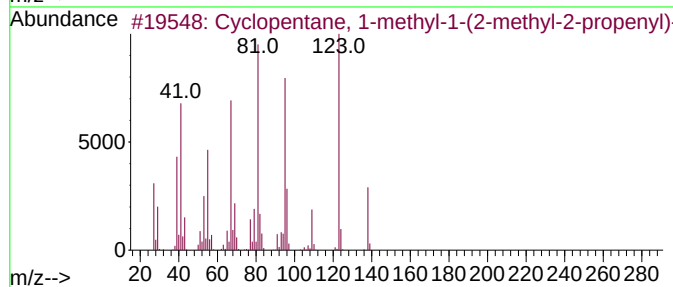
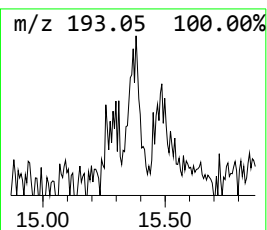
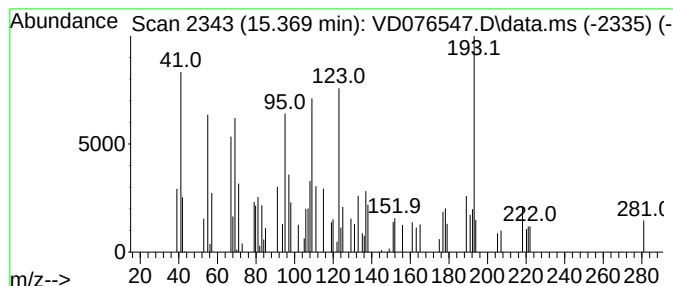
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Quant Title : SW846 8260

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

Peak Number 8 unknown15.369 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.369	32.65 ug/l	67669	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1-methyl-1-(2-meth...	138	C10H18	074764-47-9	38
2			6-Acetamido-1,4-benzodioxane	193	C10H11NO3	063546-19-0	30
3			2-Cyclopenten-1-one, 2,3,4,5-tet...	138	C9H14O	054458-61-6	25
4			Dispiro[2.2.5.0]undecan-4-one, 5...	220	C15H24O	1000152-13-8	25
5			.beta.-Alanine, N-(3-fluorobenzo...	281	C15H20FN03	1000321-93-5	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD062223\
Data File : VD076547.D
Acq On : 22 Jun 2023 19:12
Operator : KP/SY
Sample : 03365-24
Misc : 5.00G/5.0ml/MSVOA_D/SOIL
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
TP1

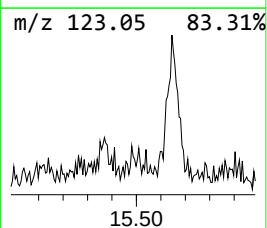
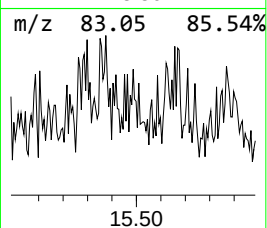
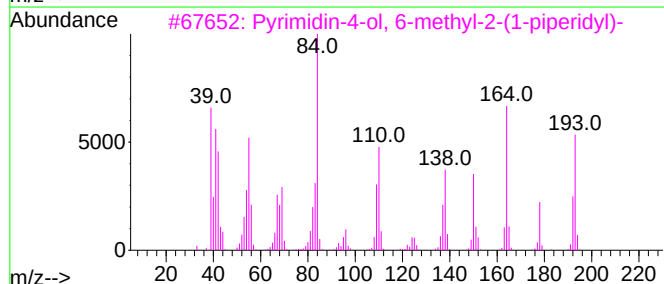
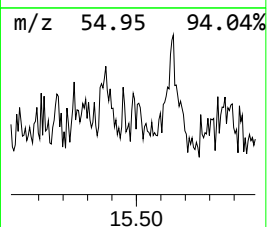
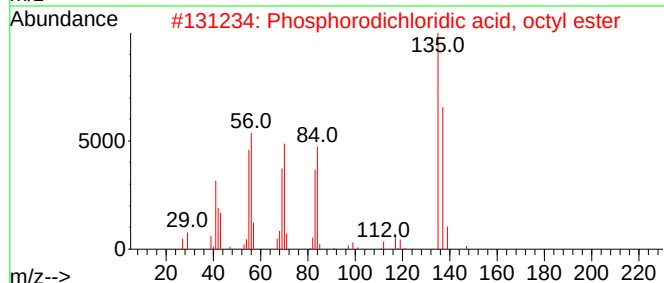
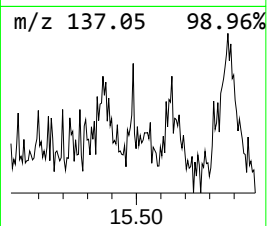
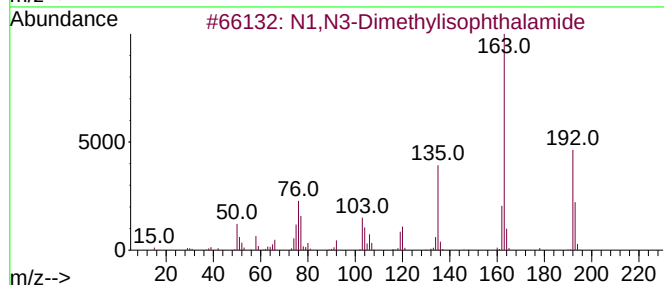
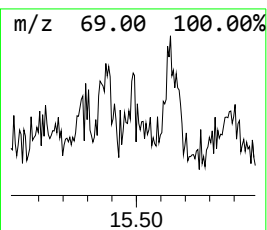
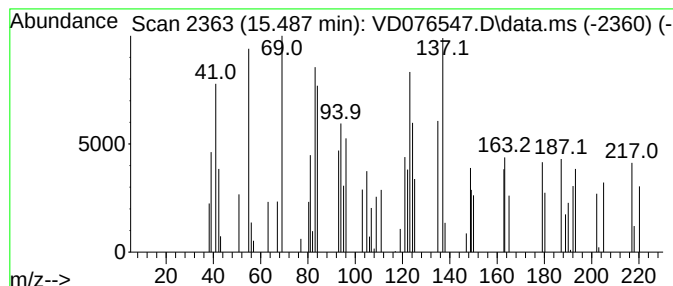
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Quant Title : SW846 8260

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

Peak Number 9 unknown15.486 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.486	8.22 ug/l	17033	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N1,N3-Dimethylisophthalamide	192	C10H12N2O2	006780-97-8	11
2			Phosphorodichloridic acid, octyl...	246	C8H17Cl2O2P	1000309-10-1	10
3			Pyrimidin-4-ol, 6-methyl-2-(1-pi...	193	C10H15N3O	042487-69-4	10
4			7-(Piperidin-1-yl)-[1,2,3,4]tetr...	220	C8H12N8	1000388-12-6	10
5			Myristoleic acid	226	C14H26O2	000544-64-9	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD062223\
Data File : VD076547.D
Acq On : 22 Jun 2023 19:12
Operator : KP/SY
Sample : 03365-24
Misc : 5.00G/5.0ml/MSVOA_D/SOIL
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
TP1

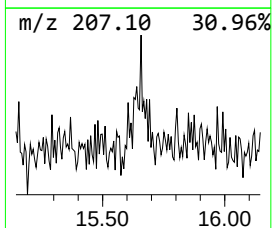
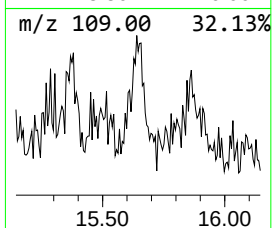
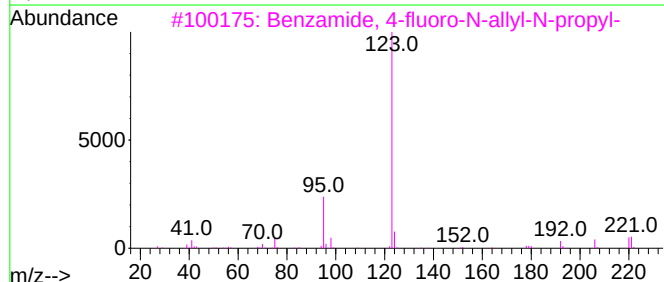
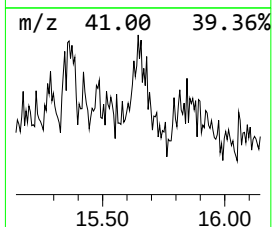
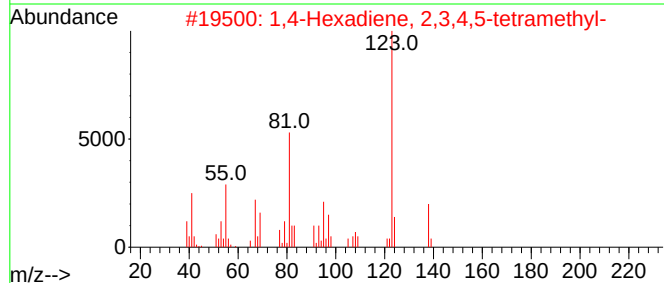
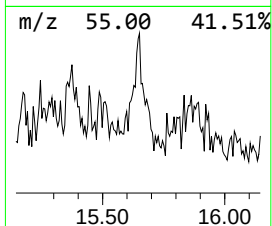
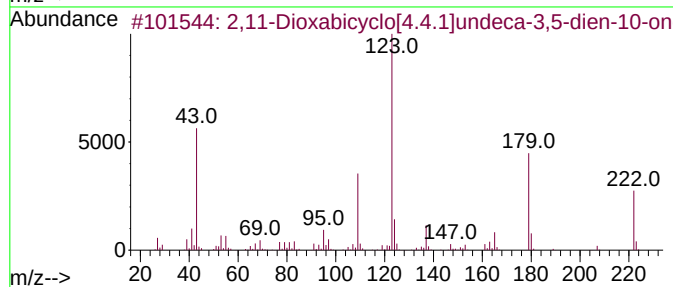
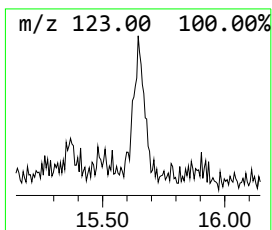
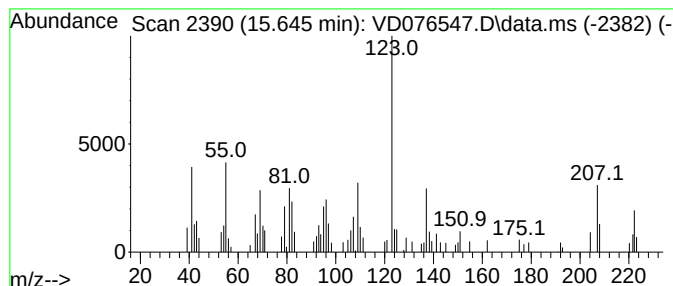
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D061623S.M
Quant Title : SW846 8260

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

Peak Number 10 unknown15.645 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.645	47.03 ug/l	97462	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	43		
2	1,4-Hexadiene, 2,3,4,5-tetramethyl-	138	C10H18	051504-54-2	41		
3	Benzamide, 4-fluoro-N-allyl-N-pr...	221	C13H16FNO	1000446-42-8	38		
4	2-Pyrimidinamine, 4,6-dimethyl-	123	C6H9N3	000767-15-7	38		
5	1,5-Diazabicyclo[4.3.0]non-5-ene	124	C7H12N2	003001-72-7	38		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD062223\
Data File : VD076547.D
Acq On : 22 Jun 2023 19:12
Operator : KP/SY
Sample : 03365-24
Misc : 5.00G/5.0ml/MSVOA_D/SOIL
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
TP1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D061623S.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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unknown13.640	13.640	76.7	ug/l	158905	4	13.516	103618	50.0
unknown13.828	13.828	17.6	ug/l	36402	4	13.516	103618	50.0
unknown14.169	14.169	5.6	ug/l	11651	4	13.516	103618	50.0
unknown15.369	15.369	32.6	ug/l	67669	4	13.516	103618	50.0
unknown15.486	15.486	8.2	ug/l	17033	4	13.516	103618	50.0
unknown15.645	15.645	47.0	ug/l	97462	4	13.516	103618	50.0