

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY052125\
 Data File : VY022376.D
 Acq On : 21 May 2025 18:39
 Operator : SY/MD
 Sample : Q2104-01
 Misc : 5.12g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 TR-06-052125

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_Y\methods\82Y051525S.M
 Title : SW846 8260

Signal : TIC: VY022376.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.879	25	26	30	rVB2	719	660	2.03%	0.269%
2	1.915	30	32	36	rBV2	533	695	2.13%	0.283%
3	1.995	44	45	49	rVB2	548	650	2.00%	0.265%
4	2.092	49	61	62	rBV2	5593	13537	41.57%	5.515%
5	2.117	63	65	67	rVV3	1391	1563	4.80%	0.637%
6	2.172	72	74	75	rVV2	1159	879	2.70%	0.358%
7	2.312	96	97	101	rVB2	743	650	2.00%	0.265%
8	2.415	112	114	117	rBV2	556	676	2.08%	0.275%
9	2.452	117	120	122	rVB3	609	679	2.09%	0.277%
10	2.495	125	127	128	rBV	638	555	1.70%	0.226%
11	2.556	134	137	140	rVB3	640	754	2.32%	0.307%
12	2.623	144	148	151	rVV3	937	1538	4.72%	0.627%
13	2.647	151	152	158	rVB3	845	659	2.02%	0.268%
14	3.147	232	234	237	rBV4	454	570	1.75%	0.232%
15	3.202	242	243	246	rVB2	700	574	1.76%	0.234%
16	3.238	246	249	250	rBV2	486	576	1.77%	0.235%
17	3.610	307	310	313	rBV	384	566	1.74%	0.231%
18	3.793	338	340	346	rVB2	770	847	2.60%	0.345%
19	3.885	351	355	359	rVB3	453	715	2.20%	0.291%
20	4.116	390	393	396	rBV3	394	560	1.72%	0.228%
21	4.464	444	450	451	rBV3	475	680	2.09%	0.277%
22	4.580	466	469	474	rVB2	476	802	2.46%	0.327%
23	5.000	536	538	542	rBV2	372	550	1.69%	0.224%
24	5.269	580	582	587	rVB2	660	1028	3.16%	0.419%
25	5.653	643	645	647	rBV2	641	531	1.63%	0.216%
26	5.848	673	677	678	rVB2	457	586	1.80%	0.239%
27	5.945	691	693	697	rVB2	409	554	1.70%	0.226%
28	6.256	741	744	748	rVB3	357	665	2.04%	0.271%
29	6.372	760	763	766	rBV3	339	548	1.68%	0.223%
30	6.671	809	812	814	rVB4	552	566	1.74%	0.231%
31	6.774	828	829	832	rBV2	618	541	1.66%	0.220%
32	6.841	836	840	845	rVB4	372	783	2.40%	0.319%
33	7.646	963	972	977	rBV6	2247	6541	20.09%	2.665%
34	7.719	977	984	992	rVB4	7666	18838	57.85%	7.674%
35	8.067	1032	1041	1049	rBV3	4607	10682	32.81%	4.352%
36	8.158	1055	1056	1060	rVB3	627	755	2.32%	0.308%

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37	8.244	1069	1070	1075	rBV2	488	666	2.05%	0.271%
38	8.622	1126	1132	1138	rBV2	12711	25615	78.67%	10.435%
39	8.932	1178	1183	1188	rBV2	550	889	2.73%	0.362%
40	9.262	1235	1237	1241	rBV3	518	548	1.68%	0.223%
41	9.475	1269	1272	1275	rVV2	425	599	1.84%	0.244%
42	9.634	1294	1298	1302	rBV2	492	884	2.71%	0.360%
43	10.115	1370	1377	1382	rVV	18080	32561	100.00%	13.265%
44	10.152	1382	1383	1388	rVB3	793	1043	3.20%	0.425%
45	10.249	1396	1399	1402	rBV2	601	788	2.42%	0.321%
46	10.609	1454	1458	1460	rBV2	472	642	1.97%	0.262%
47	10.676	1466	1469	1472	rBV2	381	578	1.78%	0.235%
48	11.213	1554	1557	1562	rBV4	624	916	2.81%	0.373%
49	11.316	1570	1574	1577	rVB3	656	717	2.20%	0.292%
50	11.420	1586	1591	1597	rVB	12218	21366	65.62%	8.704%
51	11.523	1606	1608	1611	rBV3	397	587	1.80%	0.239%
52	11.645	1624	1628	1634	rVV3	1456	2896	8.89%	1.180%
53	11.962	1678	1680	1685	rVB4	746	1388	4.26%	0.565%
54	12.054	1692	1695	1699	rVB5	1060	1417	4.35%	0.577%
55	12.182	1708	1716	1718	rVV6	1303	2942	9.04%	1.199%
56	12.231	1721	1724	1726	rBV2	631	648	1.99%	0.264%
57	12.279	1728	1732	1734	rBV3	604	795	2.44%	0.324%
58	12.414	1749	1754	1758	rBV3	6071	8947	27.48%	3.645%
59	12.450	1758	1760	1764	rVB3	1414	1492	4.58%	0.608%
60	12.566	1777	1779	1781	rBV	609	687	2.11%	0.280%
61	12.584	1781	1782	1787	rVB5	723	603	1.85%	0.246%
62	12.657	1790	1794	1797	rBV3	823	1310	4.02%	0.534%
63	12.731	1797	1806	1813	rBV5	4694	9152	28.11%	3.728%
64	12.792	1815	1816	1820	rVB2	1099	935	2.87%	0.381%
65	12.895	1828	1833	1836	rBV4	1051	1909	5.86%	0.778%
66	12.962	1841	1844	1847	rBV5	2094	1956	6.01%	0.797%
67	13.042	1855	1857	1861	rBV3	492	650	2.00%	0.265%
68	13.176	1877	1879	1883	rBV4	918	1241	3.81%	0.506%
69	13.243	1883	1890	1894	rVV3	1842	4010	12.32%	1.634%
70	13.291	1894	1898	1901	rVV2	664	1056	3.24%	0.430%
71	13.322	1901	1903	1904	rVV2	783	842	2.59%	0.343%
72	13.352	1904	1908	1912	rVV2	4113	7830	24.05%	3.190%
73	13.383	1912	1913	1917	rVB2	1828	1380	4.24%	0.562%
74	13.493	1927	1931	1933	rVB4	787	1041	3.20%	0.424%
75	13.548	1936	1940	1942	rVV3	703	788	2.42%	0.321%
76	13.669	1954	1960	1966	rBV8	2139	5160	15.85%	2.102%

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77	13.718	1966	1968	1970	rVV2	949	933	2.87%	0.380%
78	13.773	1976	1977	1983	rBV4	668	923	2.83%	0.376%
79	13.840	1983	1988	1989	rBV4	684	916	2.81%	0.373%
80	13.871	1989	1993	1994	rVV3	698	992	3.05%	0.404%
81	13.895	1995	1997	2001	rVB4	1287	1350	4.15%	0.550%
82	13.932	2001	2003	2005	rBV3	637	573	1.76%	0.233%
83	13.999	2011	2014	2021	rBV6	1057	2168	6.66%	0.883%
84	14.169	2039	2042	2049	rVB7	974	1957	6.01%	0.797%
85	14.255	2055	2056	2060	rBV2	596	656	2.01%	0.267%
86	14.340	2067	2070	2075	rVB4	926	1302	4.00%	0.530%
87	14.395	2078	2079	2082	rVB3	685	544	1.67%	0.222%
88	14.608	2111	2114	2118	rVB3	1258	1186	3.64%	0.483%
89	14.688	2125	2127	2131	rBV2	533	603	1.85%	0.246%
90	14.755	2133	2138	2141	rBV	774	1180	3.62%	0.481%
91	14.986	2173	2176	2178	rBV2	577	608	1.87%	0.248%
92	15.279	2221	2224	2227	rBV2	605	870	2.67%	0.354%
93	15.340	2232	2234	2239	rVB3	756	897	2.75%	0.365%
94	15.389	2239	2242	2246	rBV2	564	894	2.75%	0.364%
95	15.578	2270	2273	2277	rVB2	569	861	2.64%	0.351%
96	16.102	2357	2359	2361	rBV	921	641	1.97%	0.261%
97	16.181	2370	2372	2376	rVB3	720	940	2.89%	0.383%
98	16.218	2376	2378	2381	rBV2	949	896	2.75%	0.365%
99	16.376	2401	2404	2407	rBV3	790	937	2.88%	0.382%
100	16.437	2409	2414	2415	rVB4	378	615	1.89%	0.251%

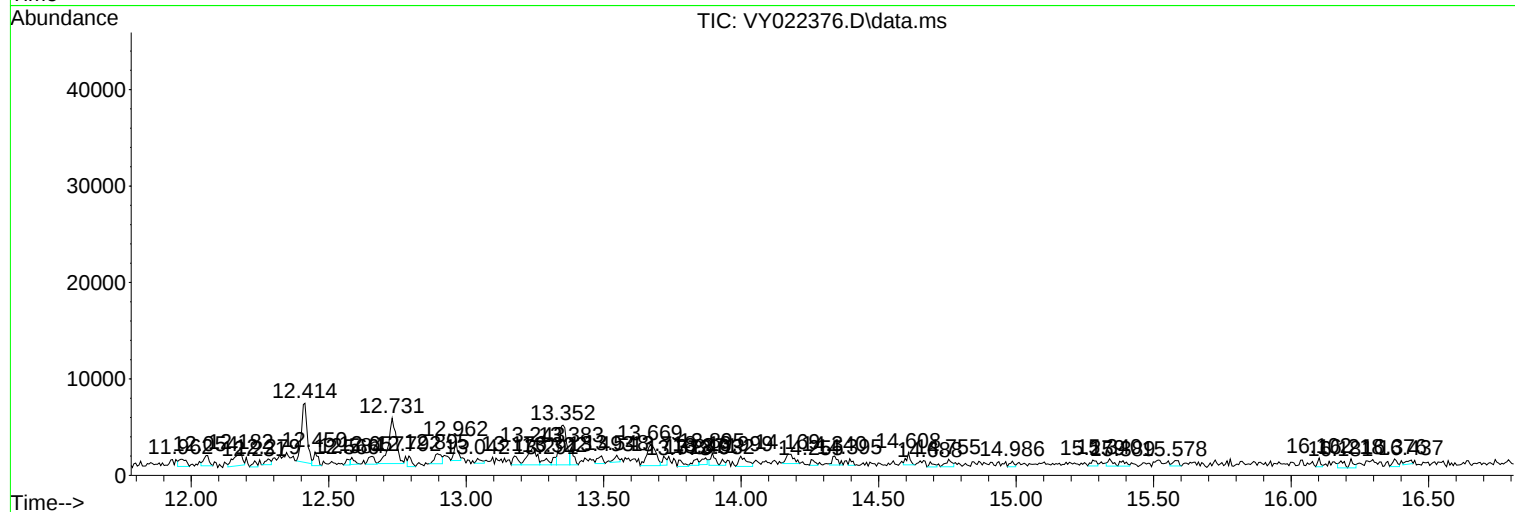
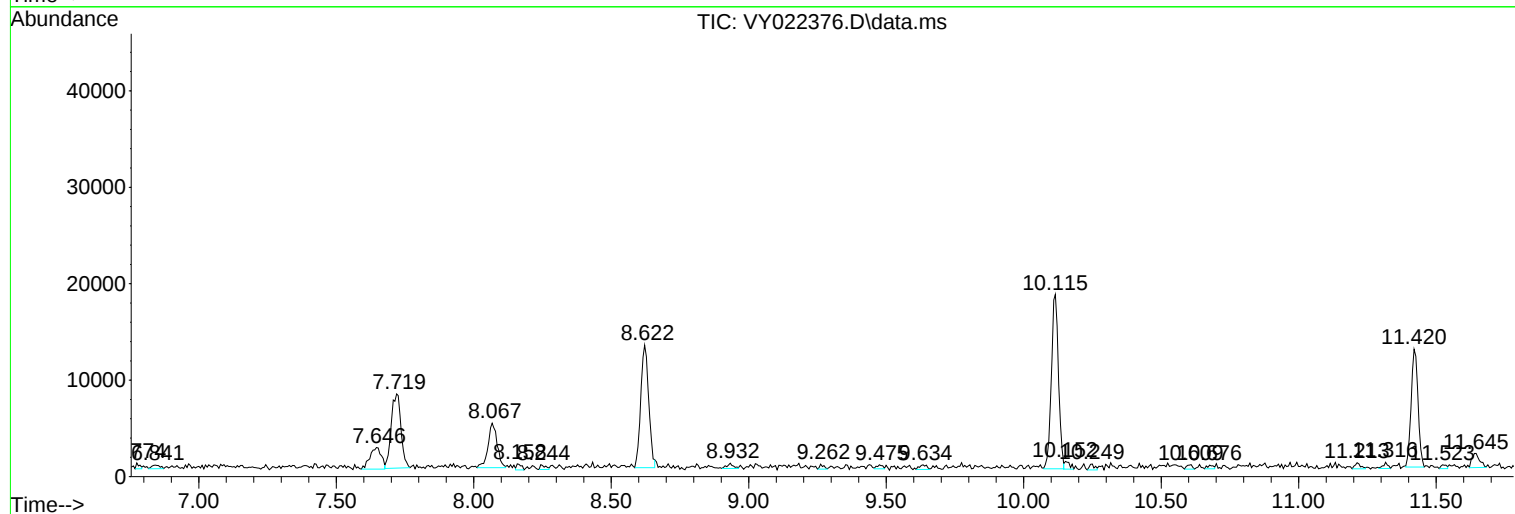
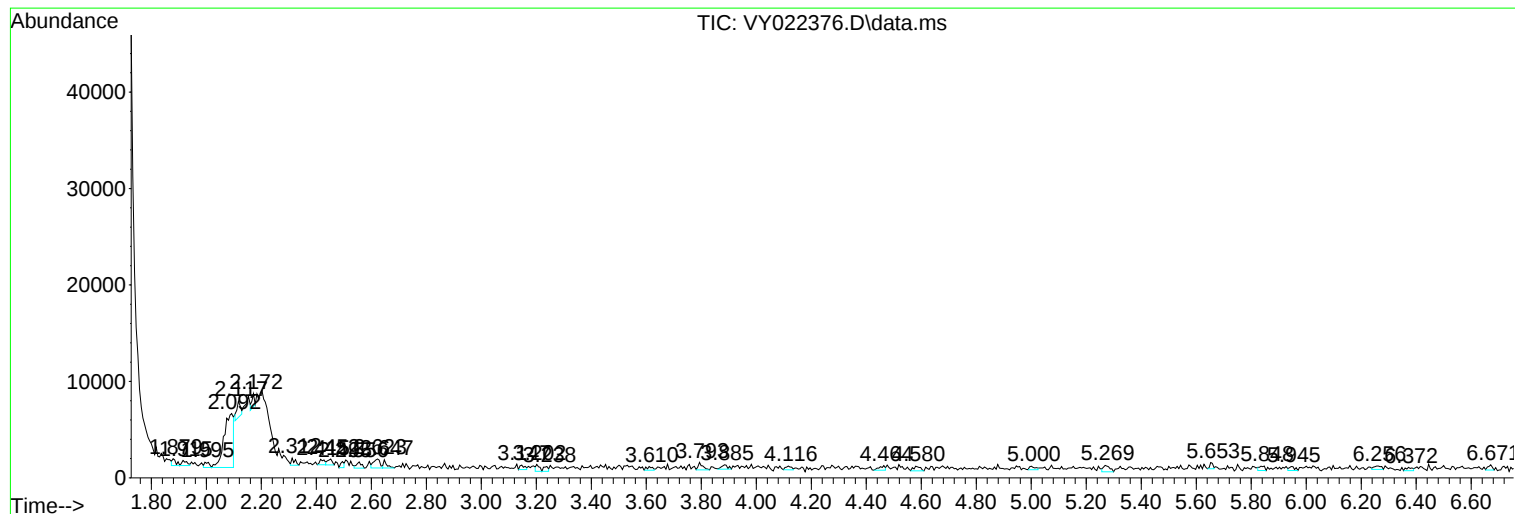
Sum of corrected areas: 245469

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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TR-06-052125

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051525S.M
Quant Title : SW846 8260

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



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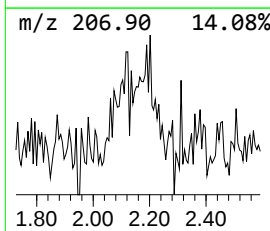
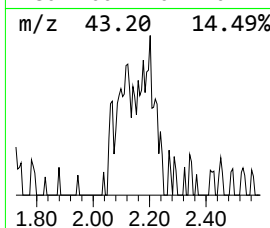
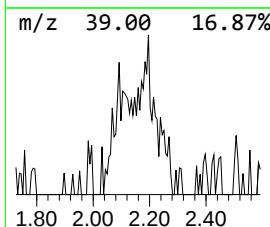
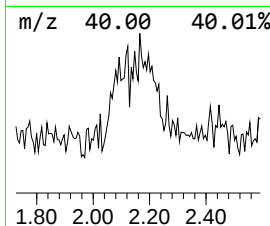
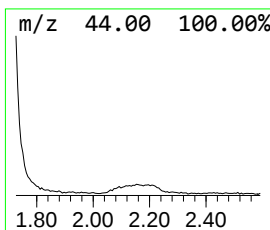
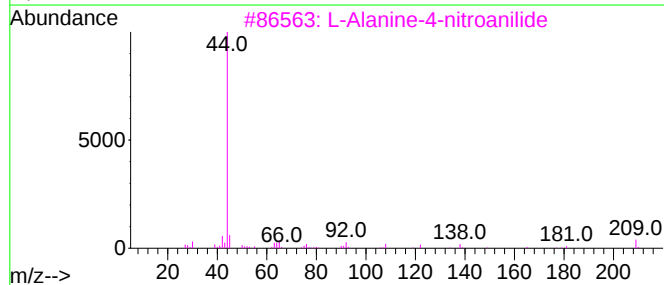
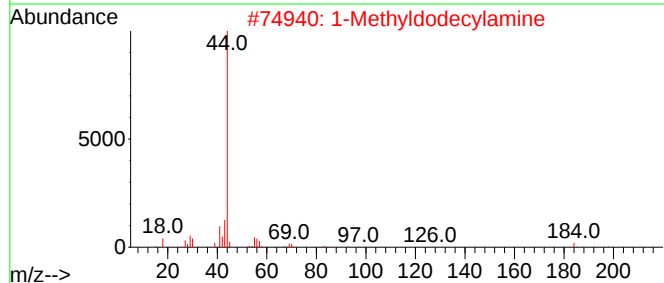
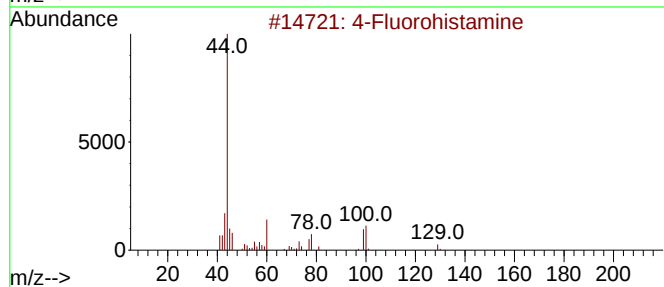
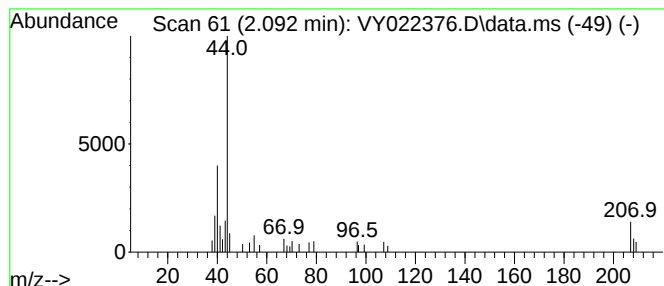
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051525S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.092 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.092	35.93 ug/l	13537	Pentafluorobenzene	7.707

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Fluorohistamine	129	C5H8FN3	049872-60-8	33
2		1-Methyldodecylamine	199	C13H29N	013205-57-7	28
3		L-Alanine-4-nitroanilide	209	C9H11N3O3	001668-13-9	9
4		Ethylamine, 1-(2-thenyl)-, hydro...	141	C7H11NS	053632-92-1	9
5		5-Aminoisoxazole	84	C3H4N2O	014678-05-8	9



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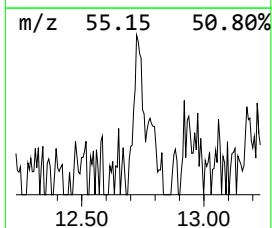
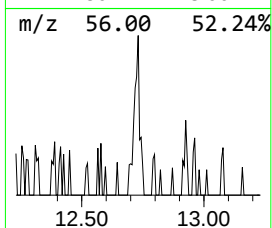
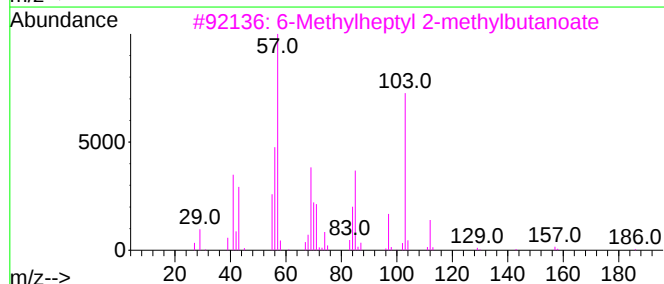
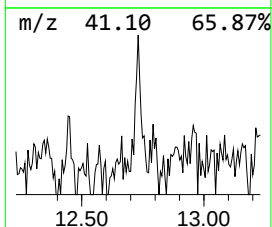
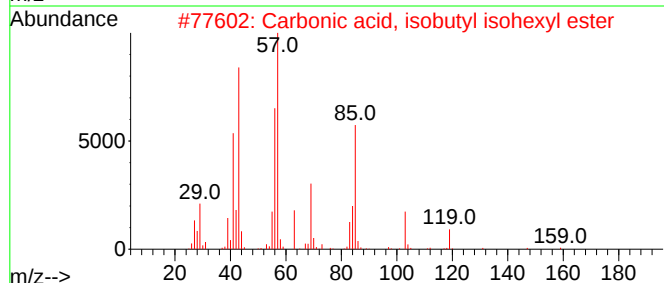
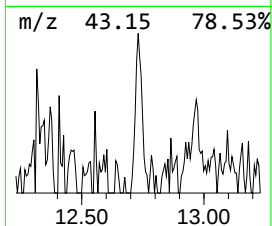
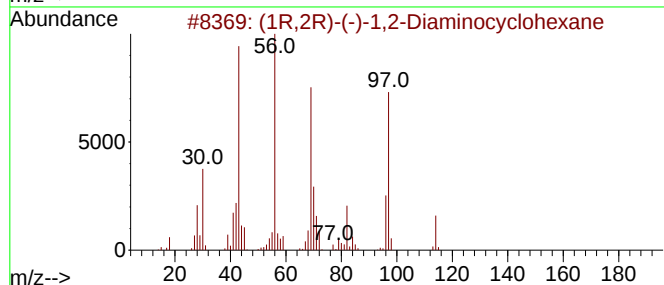
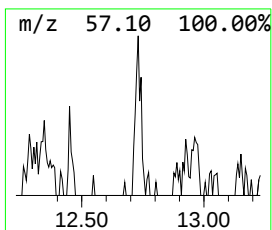
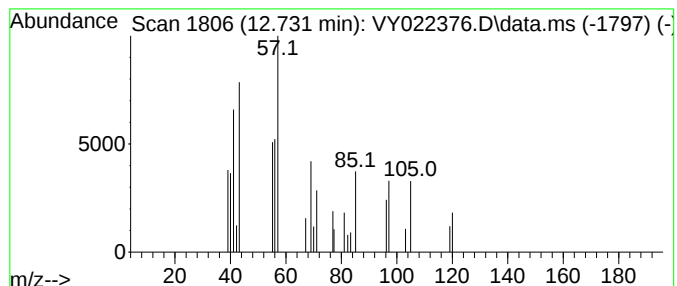
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown12.731 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.731	58.44 ug/l	9152	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R,2R)-(-)-1,2-Diaminocyclohexane	114	C6H14N2	020439-47-8	27		
2	Carbonic acid, isobutyl isohexyl...	202	C11H22O3	1000314-60-3	27		
3	6-Methylheptyl 2-methylbutanoate	214	C13H26O2	117421-31-5	17		
4	Acetic acid, trichloro-, nonyl e...	288	C11H19Cl3O2	065611-32-7	16		
5	Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	14		



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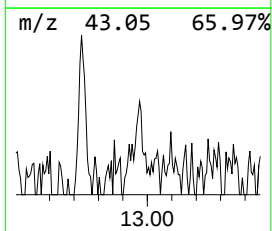
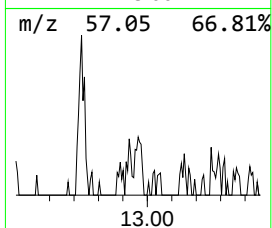
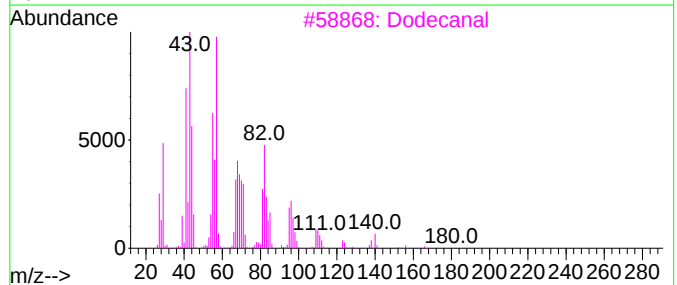
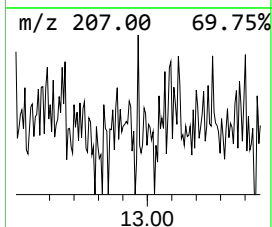
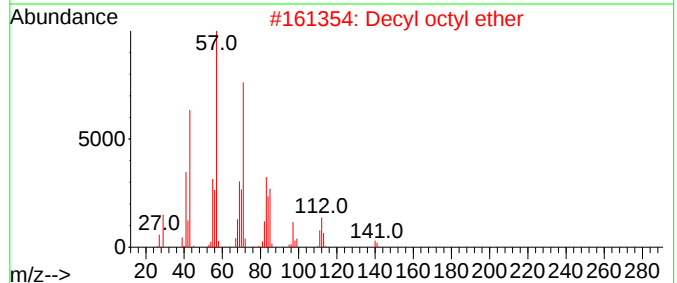
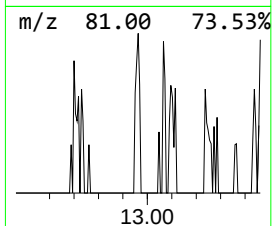
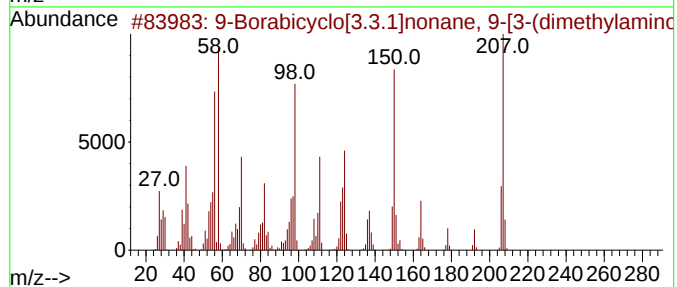
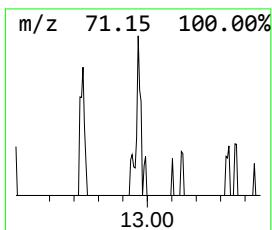
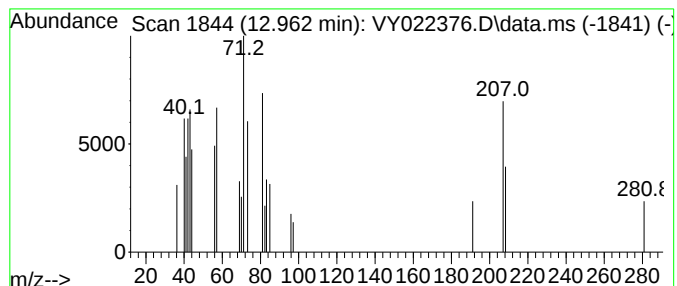
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051525S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown12.962 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.962	12.49 ug/l	1956	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Borabicyclo[3.3.1]nonane, 9-[3...	207	C13H26BN	1000160-35-2	11		
2	Decyl octyl ether	270	C18H38O	1000406-38-3	10		
3	Dodecanal	184	C12H24O	000112-54-9	10		
4	Urea, 1-methylcyclopropyl-	114	C5H10N2O	058102-14-0	10		
5	Hexyl octyl ether	214	C14H30O	017071-54-4	9		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY052125\
Data File : VY022376.D
Acq On : 21 May 2025 18:39
Operator : SY/MD
Sample : Q2104-01
Misc : 5.12g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TR-06-052125

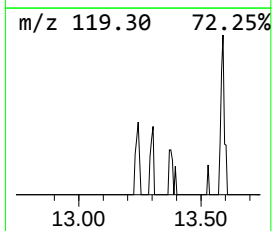
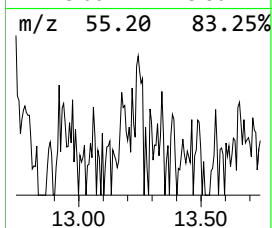
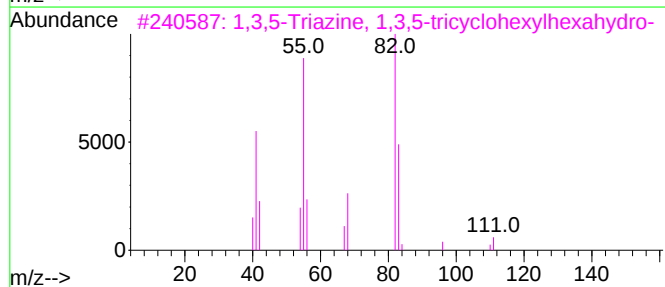
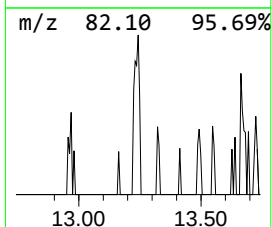
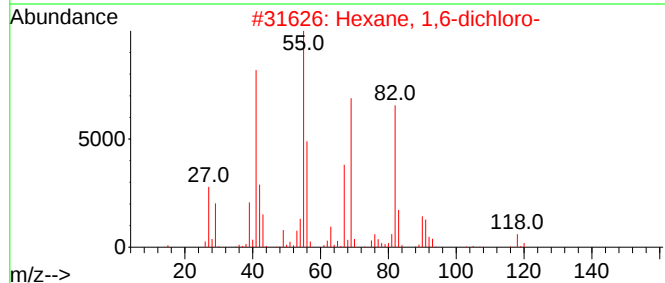
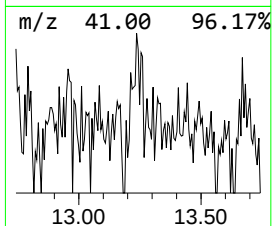
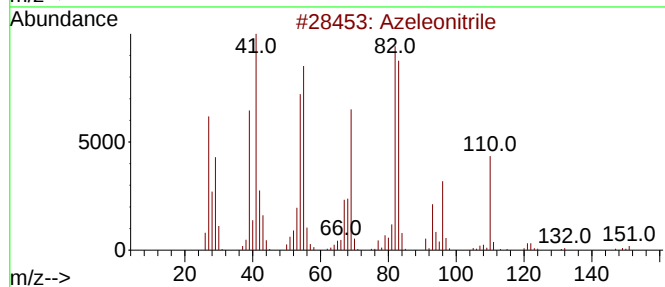
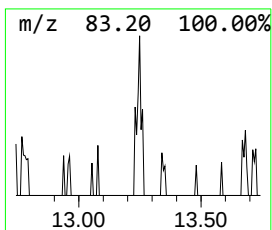
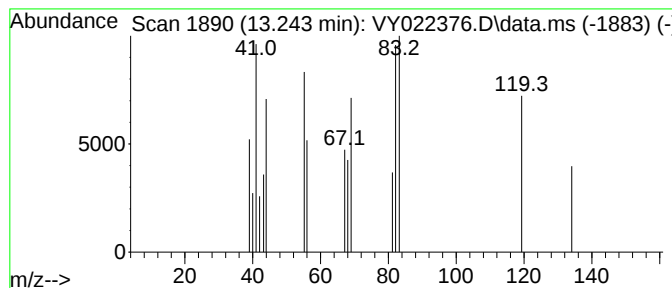
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Quant Title : SW846 8260

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

Peak Number 6 unknown13.243 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.243	25.61 ug/l	4010	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azeleonnitrile	150	C9H14N2	001675-69-0	37
2			Hexane, 1,6-dichloro-	154	C6H12Cl2	002163-00-0	35
3			1,3,5-Triazine, 1,3,5-tricyclohe...	333	C21H39N3	006281-14-7	35
4			2-Heptenal, (E)-	112	C7H12O	018829-55-5	35
5			2-Heptenal, (Z)-	112	C7H12O	057266-86-1	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY052125\
Data File : VY022376.D
Acq On : 21 May 2025 18:39
Operator : SY/MD
Sample : Q2104-01
Misc : 5.12g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 24 Sample Multiplier: 1

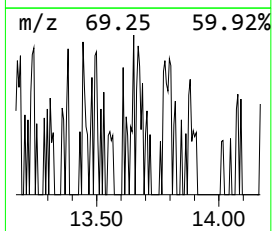
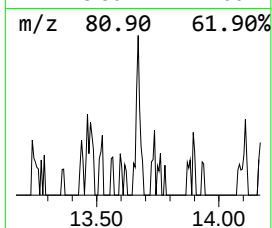
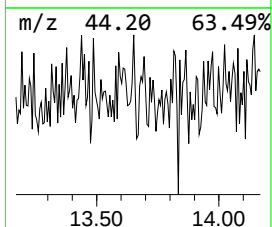
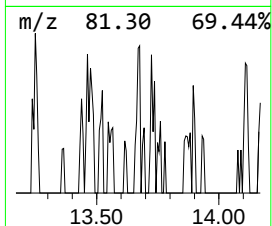
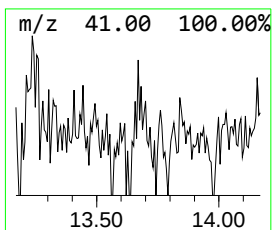
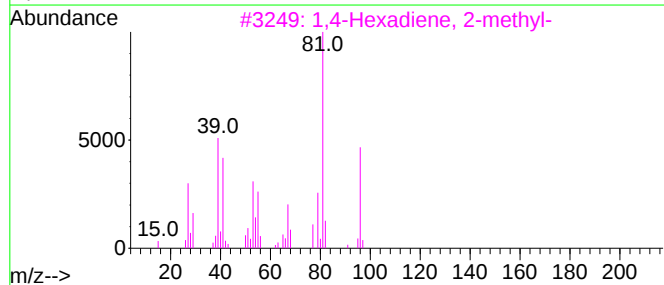
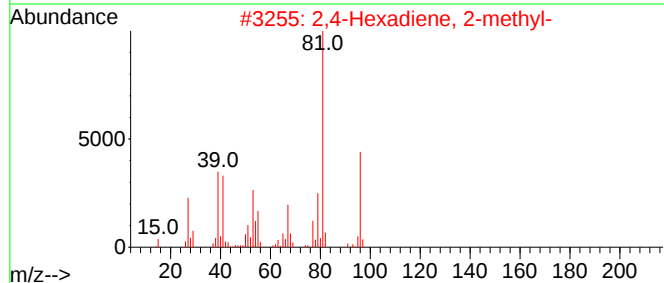
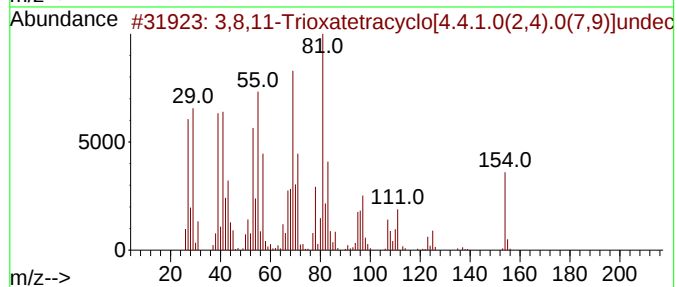
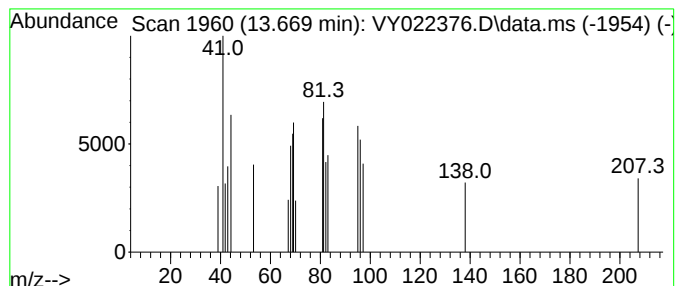
Instrument :
MSVOA_Y
ClientSampleId :
TR-06-052125

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051525S.M
Quant Title : SW846 8260

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

Peak Number 7 3,8,11-Trioxatetracyclo[4.4... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD			R.T.
13.669	32.95 ug/l	5160	1,4-Dichlorobenzene-d4			13.346
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,8,11-Trioxatetracyclo[4.4.1.0(...	154	C8H10O3		050267-11-3	64
2	2,4-Hexadiene, 2-methyl-	96	C7H12		028823-41-8	38
3	1,4-Hexadiene, 2-methyl-	96	C7H12		001119-14-8	38
4	1,4-Hexadiene, 4-methyl-	96	C7H12		001116-90-1	38
5	2,4-Hexadiene, 3-methyl-	96	C7H12		028823-42-9	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY052125\
Data File : VY022376.D
Acq On : 21 May 2025 18:39
Operator : SY/MD
Sample : Q2104-01
Misc : 5.12g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TR-06-052125

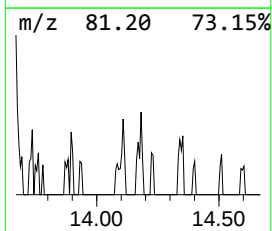
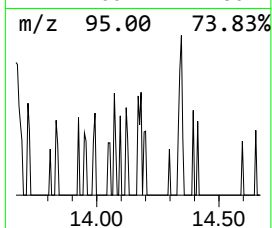
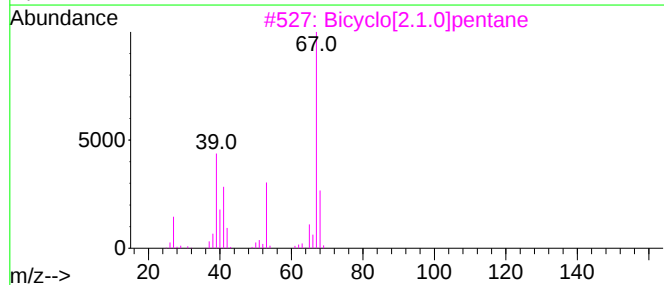
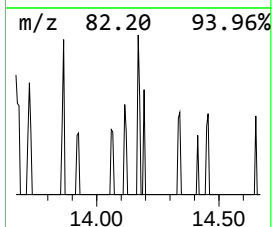
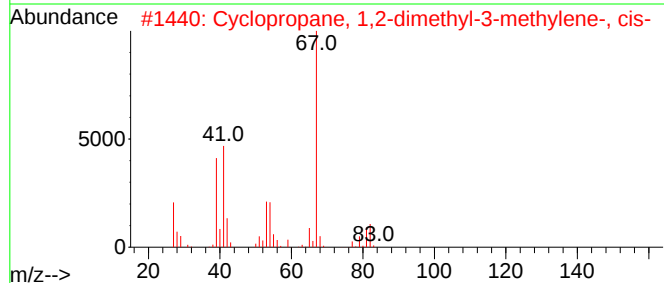
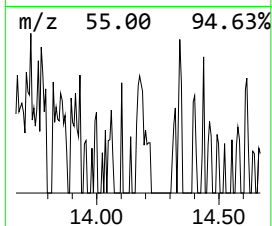
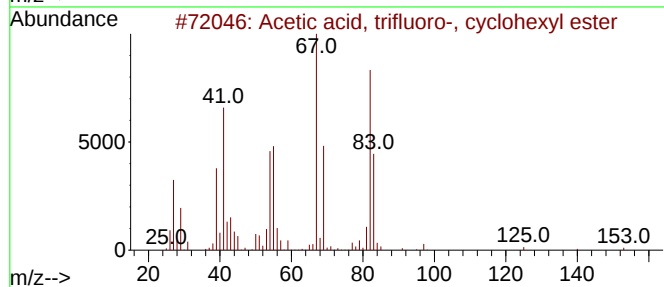
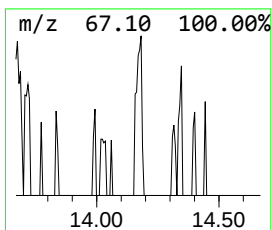
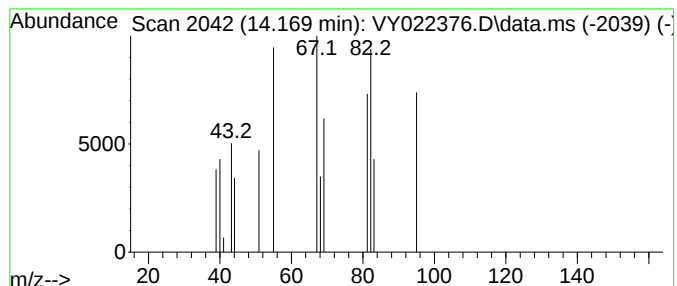
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Quant Title : SW846 8260

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

Peak Number 10 unknown14.169 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.169	12.50 ug/l	1957	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, trifluoro-, cyclohe...	196	C8H11F3O2	001549-45-7	25
2			Cyclopropane, 1,2-dimethyl-3-met...	82	C6H10	004866-55-1	9
3			Bicyclo[2.1.0]pentane	68	C5H8	000185-94-4	9
4			Cyclopropane, methylmethylene-	68	C5H8	018631-84-0	9
5			Cyclopentene	68	C5H8	000142-29-0	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY052125\
Data File : VY022376.D
Acq On : 21 May 2025 18:39
Operator : SY/MD
Sample : Q2104-01
Misc : 5.12g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TR-06-052125

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051525S.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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unknown12.731	12.731	58.4	ug/l	9152	4	13.346	7830	50.0
unknown12.962	12.962	12.5	ug/l	1956	4	13.346	7830	50.0
unknown13.243	13.243	25.6	ug/l	4010	4	13.346	7830	50.0
3,8,11-Trioxate...	13.669	33.0	ug/l	5160	4	13.346	7830	50.0
unknown14.169	14.169	12.5	ug/l	1957	4	13.346	7830	50.0