

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY111721\
 Data File : VY006787.D
 Acq On : 17 Nov 2021 14:44
 Operator : SY/MD
 Sample : M4695-03
 Misc : 5.00G/5ML/MSVOA_Y/SOIL
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 289

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\82Y111521S.M
 Title : SW846 8260

Signal : TIC: VY006787.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.040	34	36	40	rBV3	1002	1296	1.85%	0.428%
2	2.656	136	137	143	rVB3	934	1525	2.18%	0.504%
3	3.948	347	349	356	rVB4	560	880	1.26%	0.291%
4	4.722	471	476	482	rVB3	654	1438	2.05%	0.475%
5	7.728	962	969	974	rBV3	2107	4806	6.86%	1.587%
6	7.795	974	980	989	rVB3	3877	8187	11.69%	2.703%
7	8.143	1027	1037	1044	rVB3	4485	13814	19.72%	4.562%
8	8.697	1120	1128	1134	rVV	6157	11836	16.89%	3.908%
9	9.685	1285	1290	1292	rBV3	416	755	1.08%	0.249%
10	10.185	1363	1372	1379	rBV2	10835	19574	27.94%	6.464%
11	10.356	1397	1400	1403	rVB3	812	918	1.31%	0.303%
12	10.398	1403	1407	1409	rVB4	554	719	1.03%	0.237%
13	10.575	1432	1436	1437	rBV3	1143	1551	2.21%	0.512%
14	10.734	1458	1462	1464	rBV5	636	910	1.30%	0.300%
15	10.843	1478	1480	1483	rVV4	778	881	1.26%	0.291%
16	10.916	1491	1492	1495	rVB3	1036	720	1.03%	0.238%
17	10.947	1495	1497	1502	rBV5	821	1581	2.26%	0.522%
18	11.069	1513	1517	1519	rBV5	996	1377	1.97%	0.455%
19	11.233	1541	1544	1547	rBV5	738	1512	2.16%	0.499%
20	11.325	1554	1559	1563	rBV8	2581	6479	9.25%	2.139%
21	11.398	1569	1571	1574	rBV4	599	870	1.24%	0.287%
22	11.496	1581	1587	1595	rBV	8953	16497	23.55%	5.448%
23	11.599	1602	1604	1606	rBV3	799	997	1.42%	0.329%
24	11.703	1619	1621	1625	rVB5	961	1127	1.61%	0.372%
25	11.782	1631	1634	1636	rVB4	991	1097	1.57%	0.362%
26	11.898	1650	1653	1655	rBV4	668	879	1.25%	0.290%
27	11.983	1665	1667	1669	rBV3	973	862	1.23%	0.285%
28	12.020	1671	1673	1676	rBV3	1039	1502	2.14%	0.496%
29	12.050	1676	1678	1679	rBV2	1248	857	1.22%	0.283%
30	12.136	1679	1692	1693	rBV5	9400	27428	39.15%	9.057%
31	12.343	1721	1726	1734	rBV10	2614	6435	9.18%	2.125%
32	12.489	1739	1750	1754	rBV4	12101	26749	38.18%	8.833%
33	12.812	1799	1803	1809	rVB8	1233	2456	3.51%	0.811%
34	12.922	1819	1821	1825	rVB5	1249	1670	2.38%	0.551%
35	13.142	1855	1857	1859	rBV3	1652	1621	2.31%	0.535%
36	13.221	1862	1870	1882	rVB3	6377	25975	37.07%	8.577%

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37	13.434	1895	1905	1915	rVB8	19830	70061	100.00%	23.135%
38	13.617	1928	1935	1937	rBV6	3138	6475	9.24%	2.138%
39	13.782	1953	1962	1963	rBV7	5421	10700	15.27%	3.533%
40	13.904	1979	1982	1984	rBV4	770	1008	1.44%	0.333%
41	14.099	2002	2014	2020	rBV4	2840	9705	13.85%	3.205%
42	14.300	2045	2047	2050	rBV4	730	794	1.13%	0.262%
43	14.605	2094	2097	2102	rBV6	728	1564	2.23%	0.516%
44	14.684	2107	2110	2111	rBV3	754	741	1.06%	0.245%
45	14.733	2117	2118	2121	rVB3	919	828	1.18%	0.273%
46	15.190	2190	2193	2195	rVV3	586	739	1.05%	0.244%
47	15.239	2196	2201	2204	rVV5	1031	1535	2.19%	0.507%
48	16.275	2367	2371	2375	rBV7	633	902	1.29%	0.298%

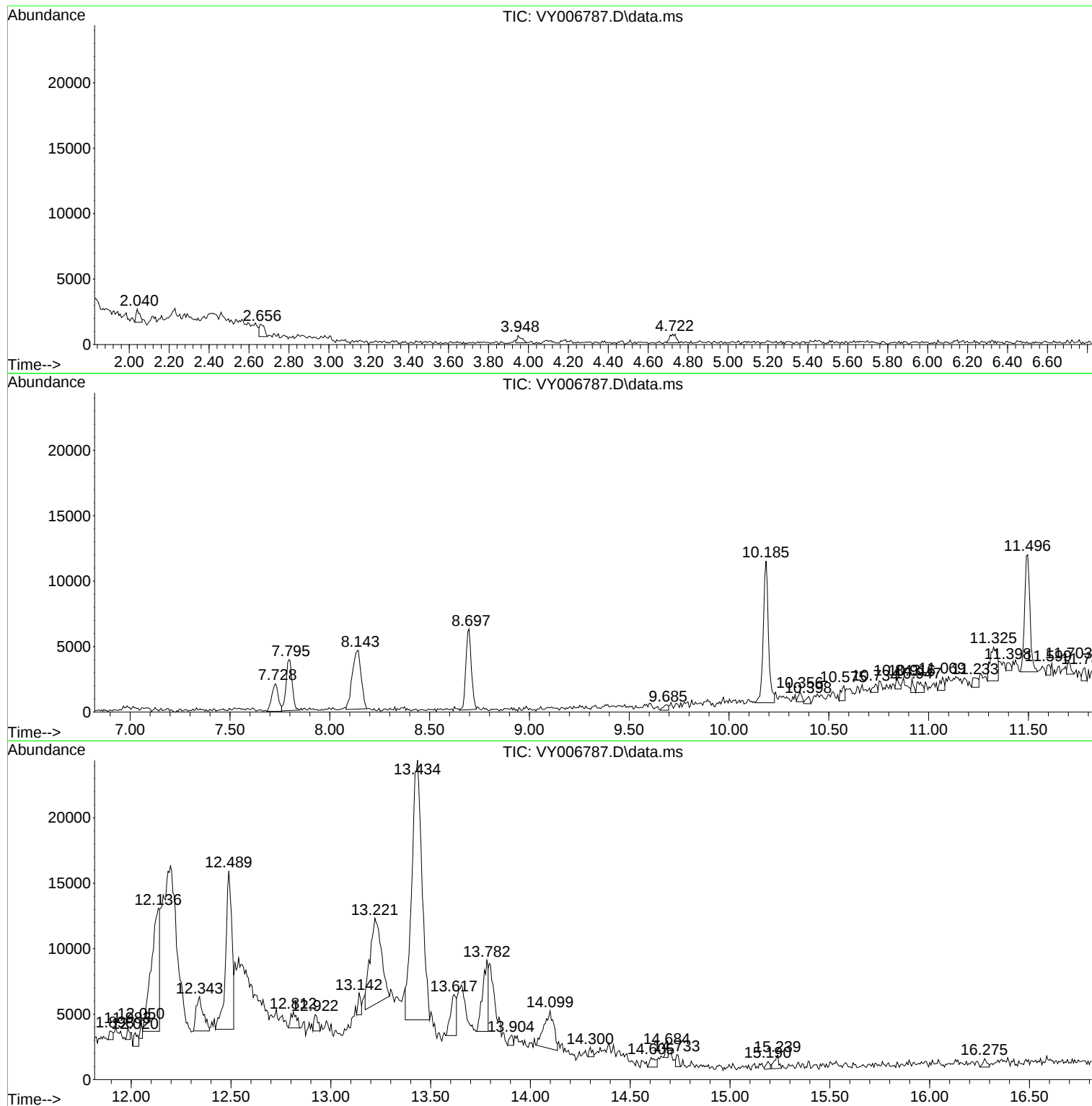
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111521S.M
Quant Title : SW846 8260

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



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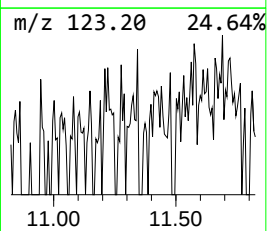
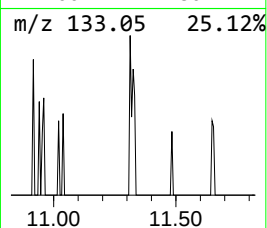
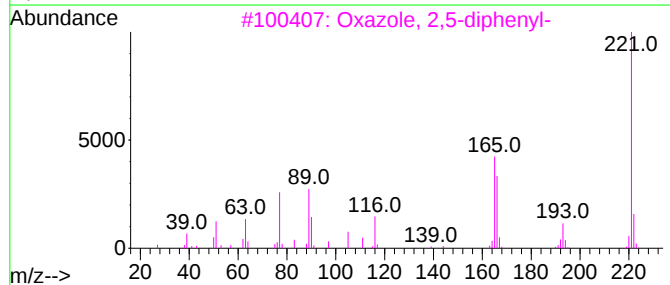
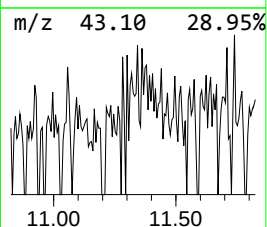
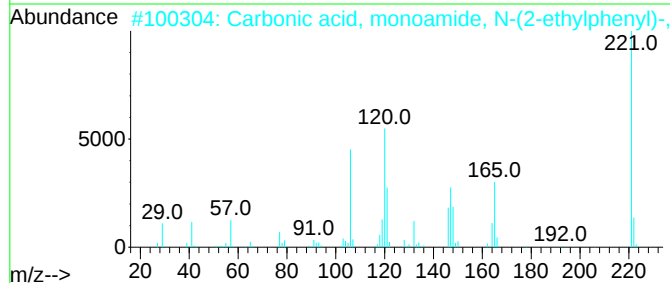
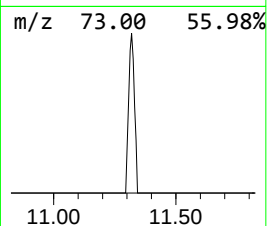
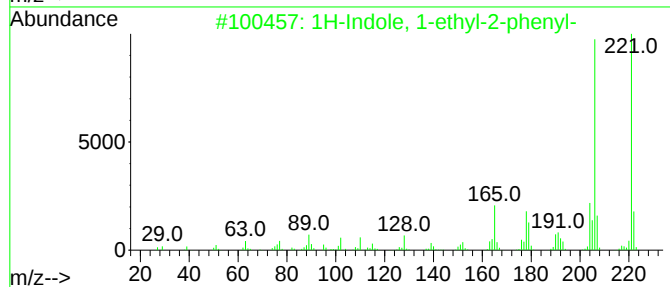
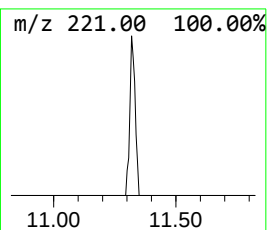
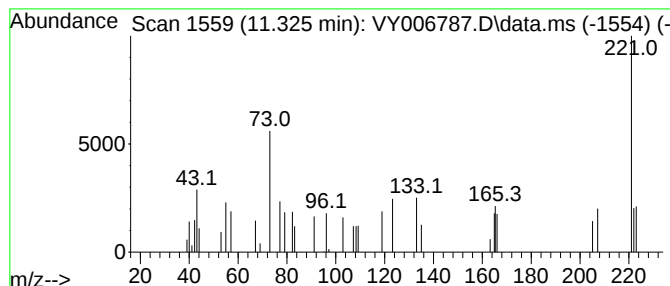
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111521S.M
Quant Title : SW846 8260

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

Peak Number 4 unknown11.325 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.325	19.64 ug/l	6479	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indole, 1-ethyl-2-phenyl-	221	C16H15N	013228-39-2	47
2			Carbonic acid, monoamide, N-(2-e...	221	C13H19NO2	1000339-98-3	43
3			Oxazole, 2,5-diphenyl-	221	C15H11NO	000092-71-7	43
4			Oxazole, 4,5-diphenyl-	221	C15H11NO	004675-18-7	37
5			2(1H)-Quinolinone, 4-phenyl-	221	C15H11NO	005855-57-2	37



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Misc : 5.00G/5ML/MSVOA_Y/SOIL
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
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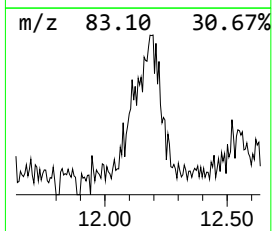
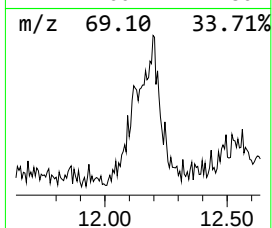
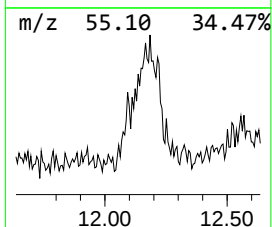
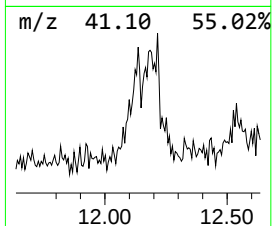
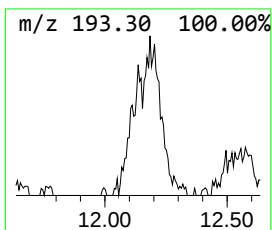
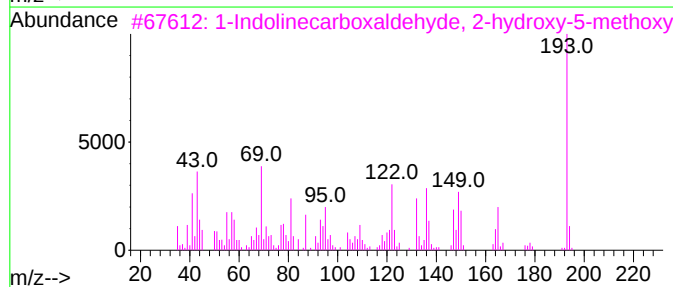
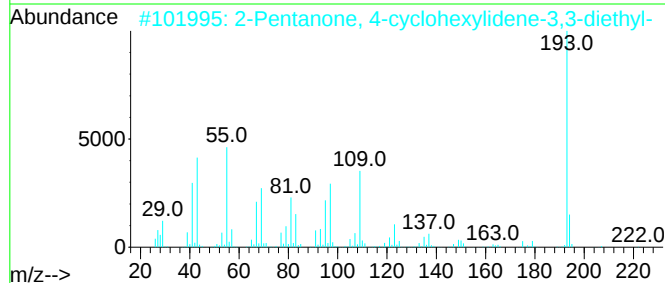
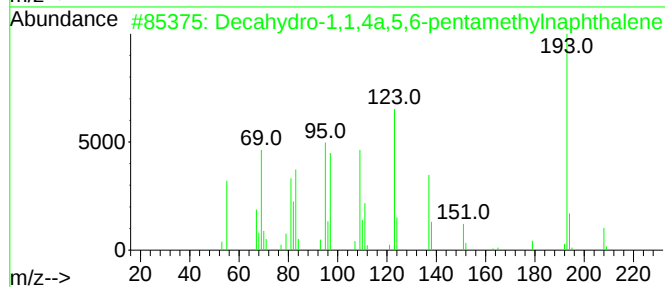
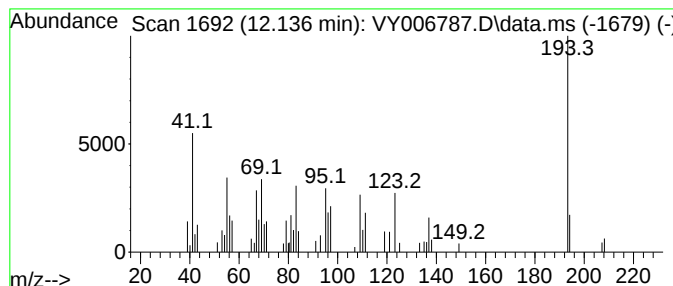
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111521S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.136	83.13 ug/l	27428	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	64
2			2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	45
3			1-Indolinecarboxaldehyde, 2-hydr...	193	C10H11NO3	013303-70-3	42
4			1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	40
5			S-Phenyl 5-(phenylthio)pentaneth...	302	C17H18OS2	1000234-40-7	37



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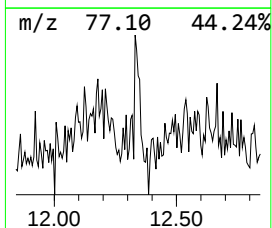
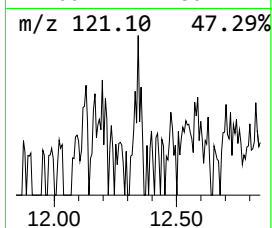
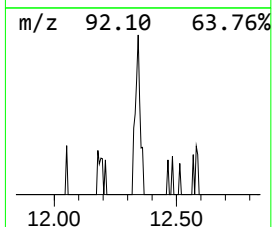
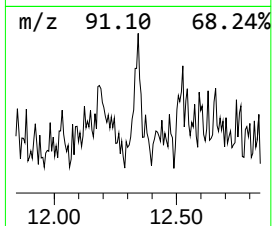
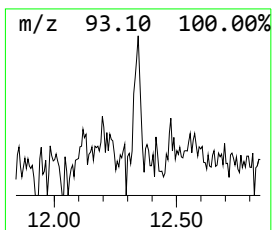
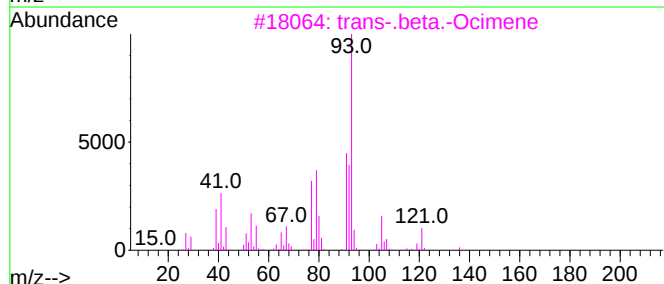
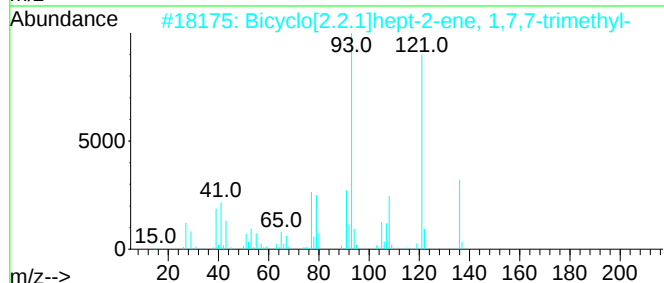
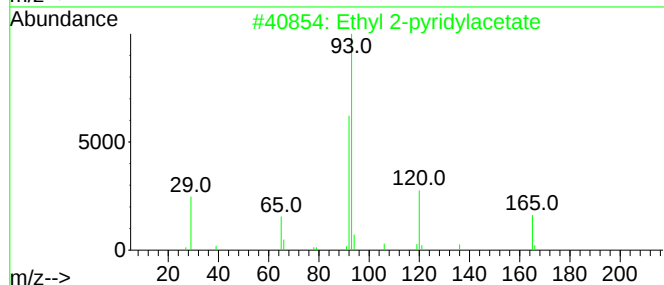
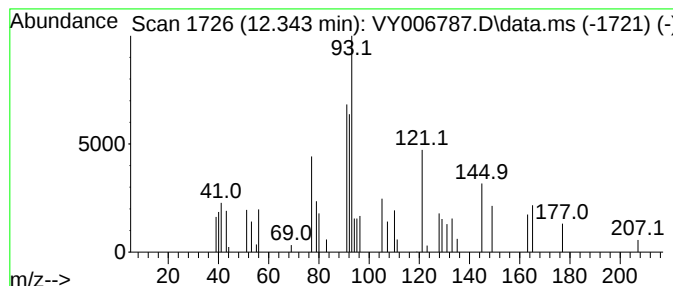
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown12.343 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.343	19.50 ug/l	6435	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl 2-pyridylacetate	165	C9H11NO2	002739-98-2	32
2			Bicyclo[2.2.1]hept-2-ene, 1,7,7-...	136	C10H16	000464-17-5	27
3			trans-.beta.-Ocimene	136	C10H16	003779-61-1	27
4			3-Carene	136	C10H16	013466-78-9	25
5			Cyclohexene, 4-(1,5-dimethyl-1,4...	204	C15H24	017627-44-0	22



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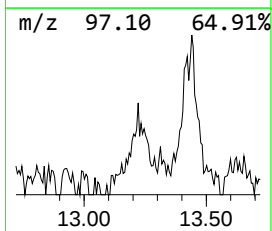
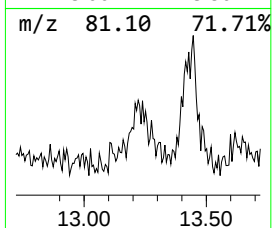
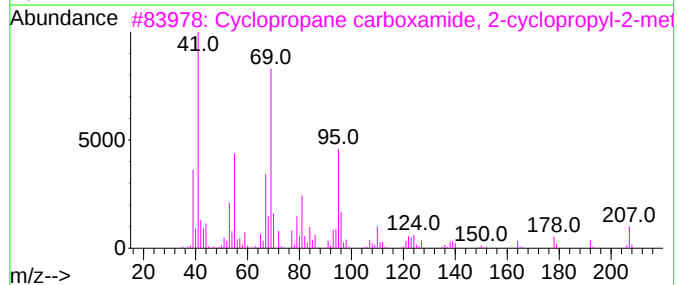
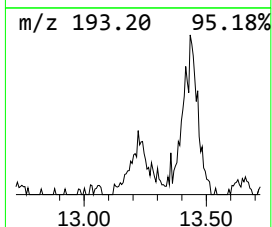
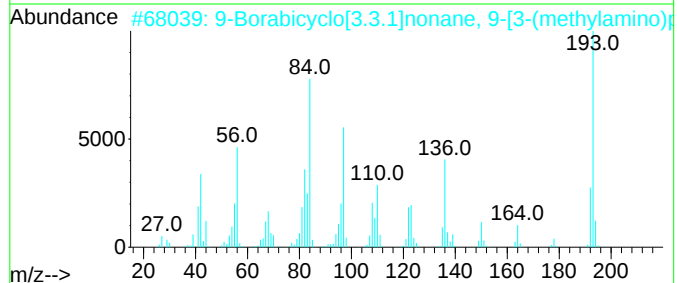
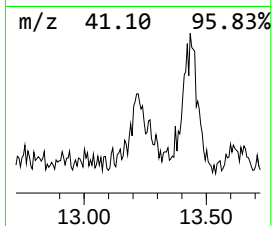
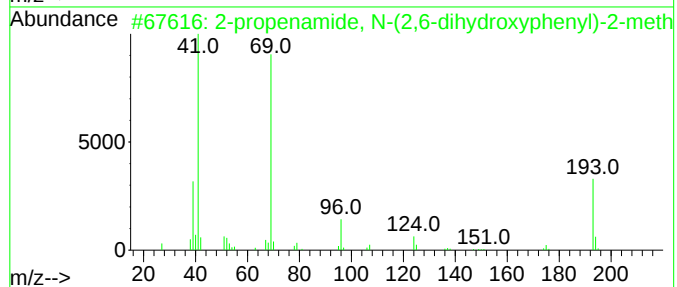
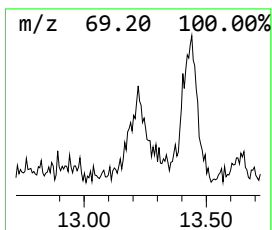
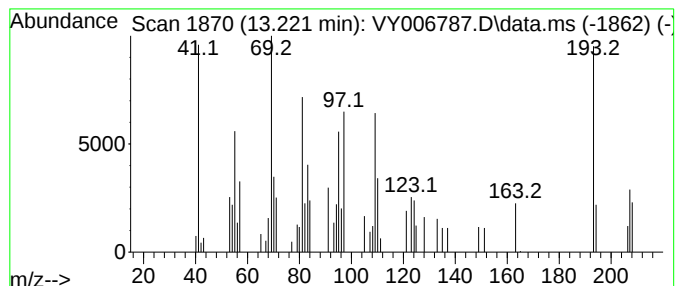
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown13.221 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.221	18.54 ug/l	25975	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-propenamide, N-(2,6-dihydroxyp...	193	C10H11NO3	1000395-98-7	38
2			9-Borabicyclo[3.3.1]nonane, 9-[3...	193	C12H24BN	1010162-56-0	30
3			Cyclopropane carboxamide, 2-cycl...	207	C13H21NO	331416-19-4	27
4			1,2-Benzenediol, 0-cyclopentanec...	206	C12H14O3	1000329-74-0	22
5			1-(10,10-Dimethyl-1,3-dioxo-3-th...	311	C16H25NO3S	1000210-42-6	22



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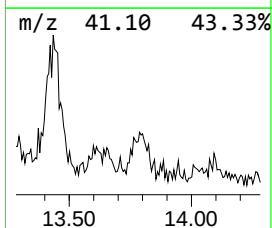
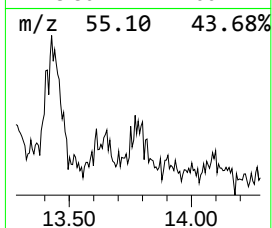
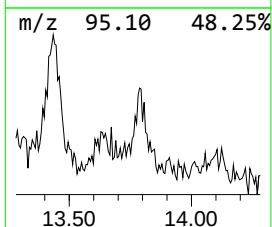
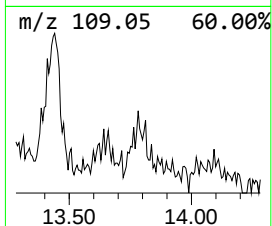
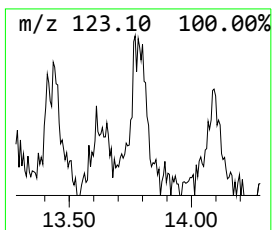
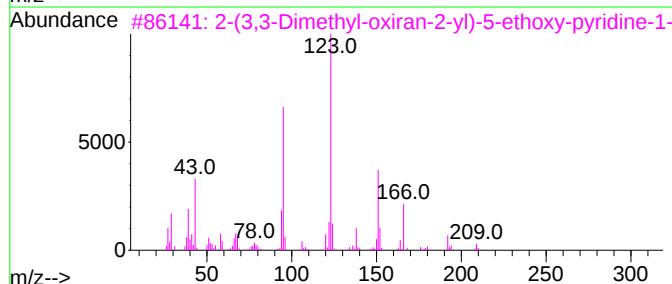
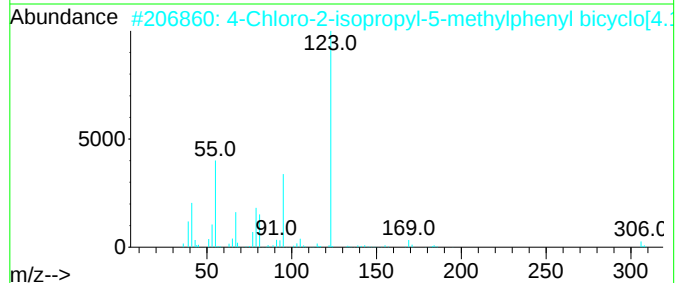
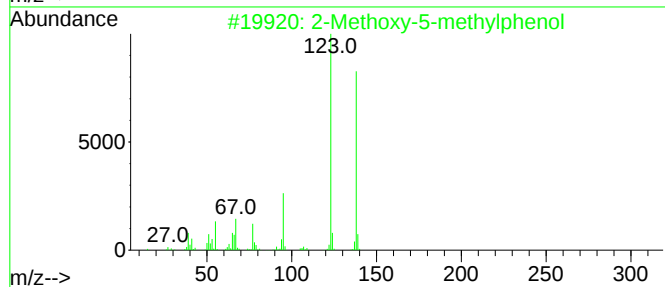
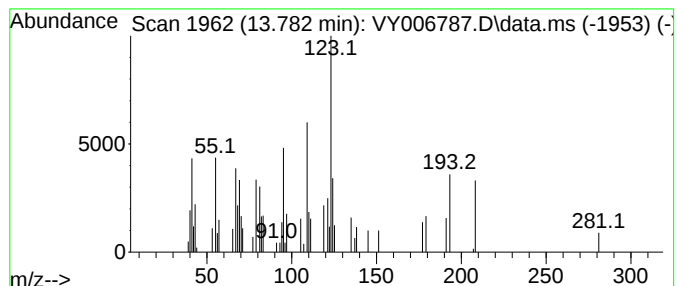
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Quant Title : SW846 8260

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

Peak Number 8 unknown13.782 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.782	7.64 ug/l	10700	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methoxy-5-methylphenol	138	C8H10O2	001195-09-1	38
2			4-Chloro-2-isopropyl-5-methylphe...	306	C18H23ClO2	321918-37-0	35
3			2-(3,3-Dimethyl-oxiran-2-yl)-5-e...	209	C11H15NO3	1000194-95-4	35
4			2-(1-Hydroxycycloheptyl)-furan	180	C11H16O2	115754-89-7	35
5			3-Fluorobenzoic acid, 2-pentadec...	350	C22H35FO2	1000280-60-7	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY111721\
Data File : VY006787.D
Acq On : 17 Nov 2021 14:44
Operator : SY/MD
Sample : M4695-03
Misc : 5.00G/5ML/MSVOA_Y/SOIL
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
289

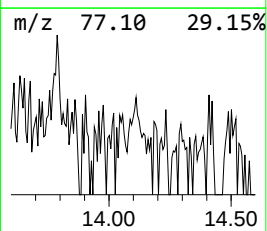
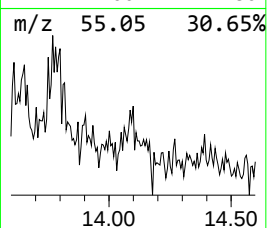
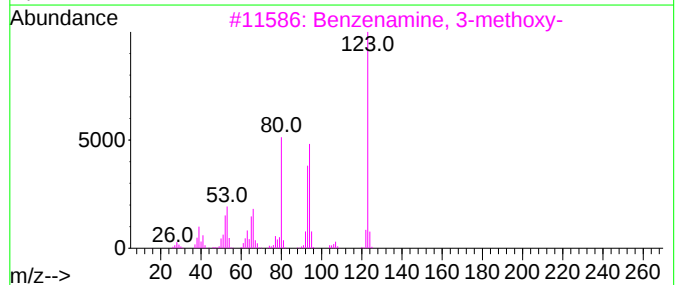
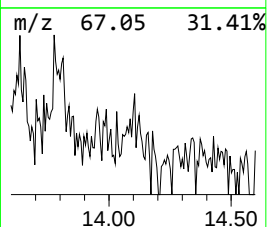
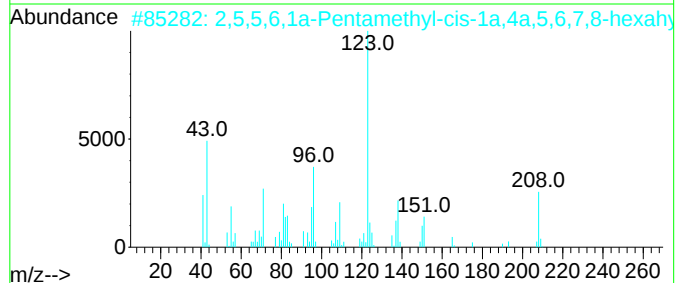
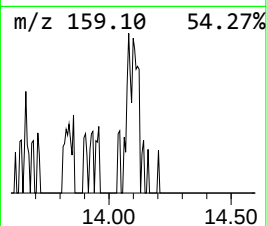
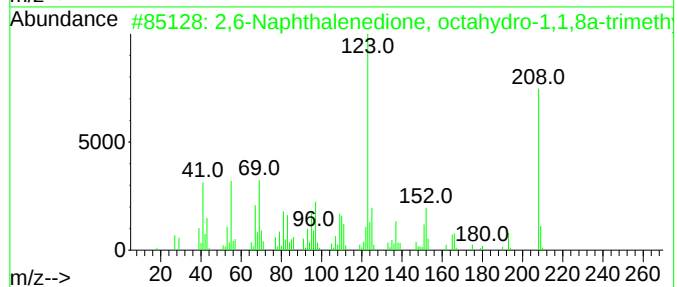
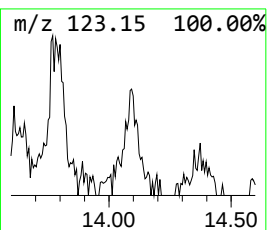
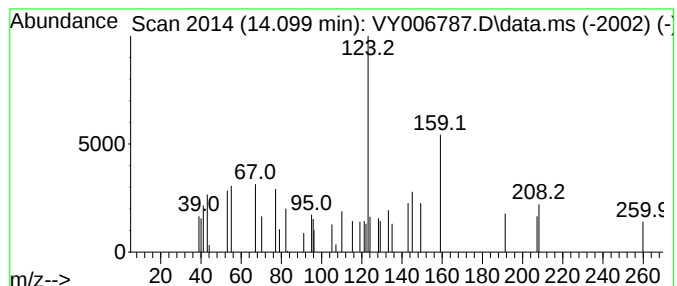
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111521S.M
Quant Title : SW846 8260

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

Peak Number 9 unknown14.099 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.099	6.93 ug/l	9705	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Naphthalenedione, octahydro-...	208	C13H20O2	057289-17-5	30		
2	2,5,5,6,1a-Pentamethyl-cis-1a,4a...	208	C14H24O	1010215-77-9	25		
3	Benzenamine, 3-methoxy-	123	C7H9NO	000536-90-3	14		
4	4-Pyrimidinamine, 2,6-dimethyl-	123	C6H9N3	000461-98-3	12		
5	3-Bromomethyl-3,6,6-trimethyl-cy...	216	C10H17Br	1000185-63-8	10		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY111721\
Data File : VY006787.D
Acq On : 17 Nov 2021 14:44
Operator : SY/MD
Sample : M4695-03
Misc : 5.00G/5ML/MSVOA_Y/SOIL
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
289

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111521S.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
unknown11.325	11.325	19.6	ug/l	6479	3	11.496	16497	50.0
Decahydro-1,1,4...	12.136	83.1	ug/l	27428	3	11.496	16497	50.0
unknown12.343	12.343	19.5	ug/l	6435	3	11.496	16497	50.0
unknown13.221	13.221	18.5	ug/l	25975	4	13.428	70061	50.0
unknown13.782	13.782	7.6	ug/l	10700	4	13.428	70061	50.0
unknown14.099	14.099	6.9	ug/l	9705	4	13.428	70061	50.0