

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071224\
 Data File : VY018805.D
 Acq On : 12 Jul 2024 18:18
 Operator : SY/MD
 Sample : P3207-07
 Misc : 5.08g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 RT-2929

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\82Y070924S.M
 Title : SW846 8260

Signal : TIC: VY018805.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.704	462	473	489	rBV2	17281	56089	5.40%	1.186%
2	5.728	632	641	655	rBV4	6237	19078	1.84%	0.403%
3	6.960	833	843	856	rBV2	7844	25829	2.49%	0.546%
4	7.710	956	966	971	rBV	62383	148772	14.32%	3.145%
5	7.783	971	978	992	rVB	99415	229082	22.05%	4.843%
6	8.130	1026	1035	1046	rBV2	56830	125731	12.10%	2.658%
7	8.679	1115	1125	1135	rBV	157537	314912	30.31%	6.658%
8	10.173	1363	1370	1380	rVB	237732	401781	38.67%	8.495%
9	10.575	1425	1436	1443	rBV	24724	44081	4.24%	0.932%
10	11.484	1578	1585	1593	rBV	210942	355764	34.24%	7.522%
11	12.227	1703	1707	1713	rVB4	7290	12028	1.16%	0.254%
12	12.331	1717	1724	1730	rBV	122942	201500	19.39%	4.260%
13	12.477	1742	1748	1756	rBV2	163665	275841	26.55%	5.832%
14	12.581	1761	1765	1768	rVB5	8358	11583	1.11%	0.245%
15	12.892	1812	1816	1822	rVB6	7130	12109	1.17%	0.256%
16	13.069	1838	1845	1851	rVB	25905	45220	4.35%	0.956%
17	13.142	1851	1857	1867	rBV	66182	107292	10.33%	2.268%
18	13.276	1874	1879	1883	rBV	14015	21545	2.07%	0.456%
19	13.343	1885	1890	1892	rBV4	11390	22840	2.20%	0.483%
20	13.422	1897	1903	1909	rVB	171379	259446	24.97%	5.485%
21	13.520	1914	1919	1921	rBV5	8494	15983	1.54%	0.338%
22	13.562	1922	1926	1927	rVV4	9231	14243	1.37%	0.301%
23	13.587	1928	1930	1934	rVB4	10814	13829	1.33%	0.292%
24	13.666	1940	1943	1946	rVB2	11563	13533	1.30%	0.286%
25	13.715	1946	1951	1955	rVB6	8962	14674	1.41%	0.310%
26	13.776	1956	1961	1963	rBV6	10042	17335	1.67%	0.367%
27	13.818	1963	1968	1973	rVV4	23225	52232	5.03%	1.104%
28	13.873	1973	1977	1980	rVB3	11514	16668	1.60%	0.352%
29	13.959	1987	1991	2005	rVB4	23611	65441	6.30%	1.384%
30	14.075	2005	2010	2015	rVV	120197	180963	17.42%	3.826%
31	14.117	2015	2017	2024	rVB4	11195	15671	1.51%	0.331%
32	14.581	2087	2093	2100	rVB	782603	1039079	100.00%	21.969%
33	14.660	2103	2106	2114	rVB8	12199	20069	1.93%	0.424%
34	14.751	2114	2121	2128	rVB	105658	168203	16.19%	3.556%
35	14.867	2134	2140	2143	rBV6	6397	11124	1.07%	0.235%
36	14.946	2147	2153	2157	rBV3	26425	54639	5.26%	1.155%

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37	15.208	2191	2196	2202	rVB	47899	77406	7.45%	1.637%
38	15.525	2241	2248	2254	rBV	48270	90713	8.73%	1.918%
39	15.599	2256	2260	2267	rVB3	18246	33730	3.25%	0.713%
40	16.001	2321	2326	2334	rBV	27989	53249	5.12%	1.126%
41	16.379	2383	2388	2390	rBV5	9604	16400	1.58%	0.347%
42	16.434	2392	2397	2409	rVB	20401	54109	5.21%	1.144%

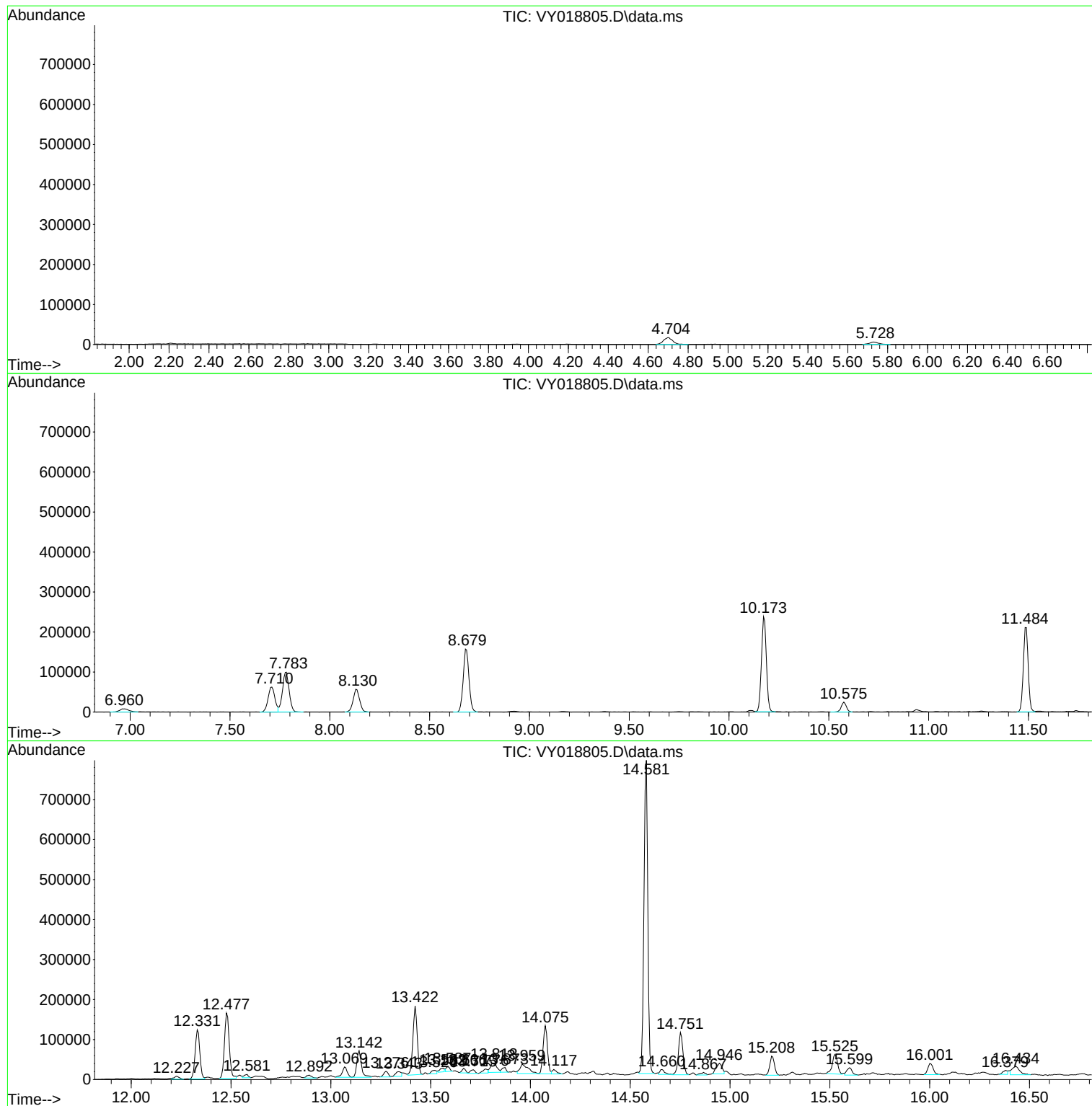
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Quant Title : SW846 8260

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



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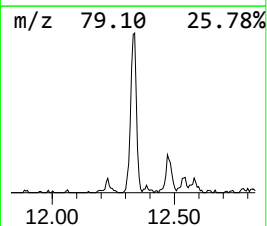
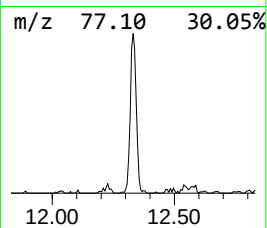
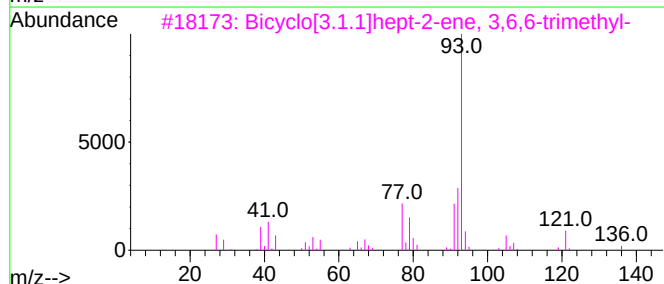
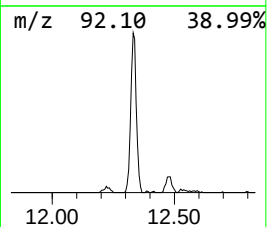
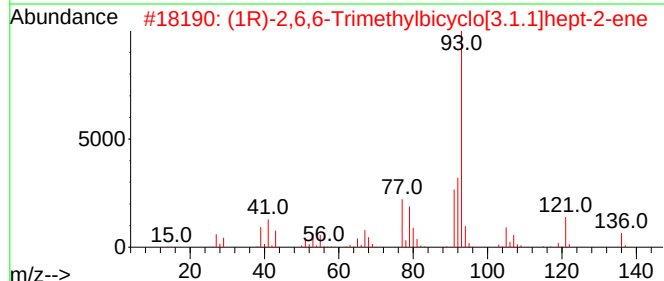
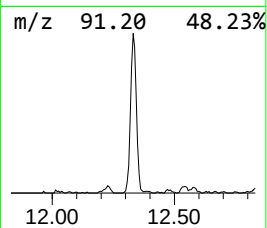
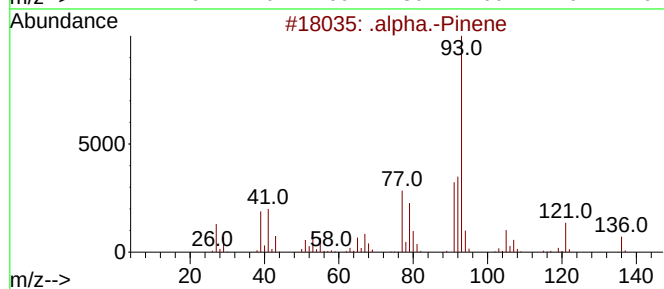
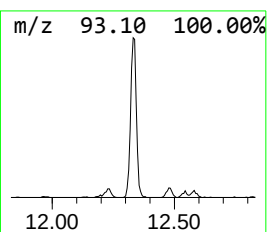
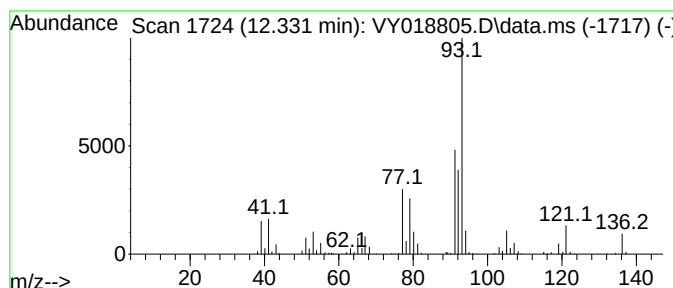
Instrument :
MSVOA_Y
ClientSampleId :
RT-2929

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070924S.M
Quant Title : SW846 8260

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

Peak Number 1 .alpha.-Pinene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.331	28.32 ug/l	201500	Chlorobenzene-d5	11.490	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Pinene	136	C10H16	000080-56-8	97
2	(1R)-2,6,6-Trimethylbicyclo[3.1...	136	C10H16	007785-70-8	94
3	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91
4	(1S)-2,6,6-Trimethylbicyclo[3.1...	136	C10H16	007785-26-4	90
5	(+)-3-Carene	136	C10H16	000498-15-7	87



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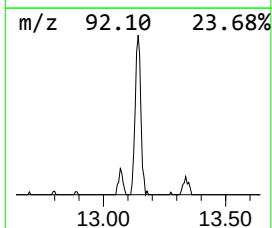
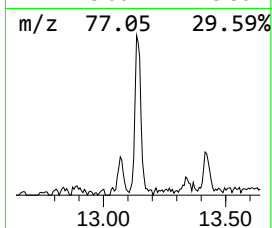
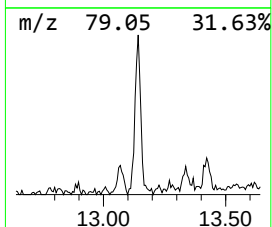
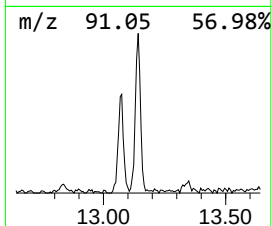
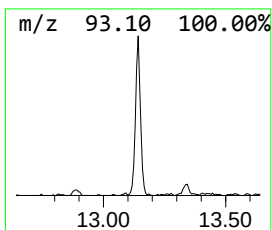
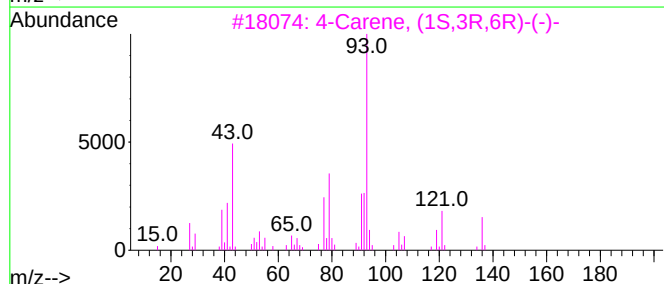
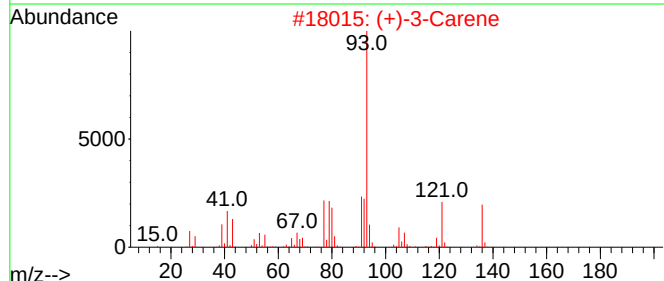
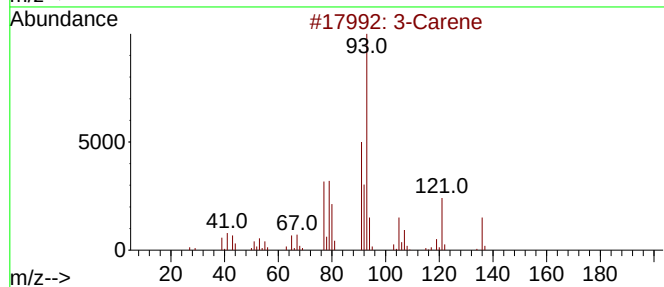
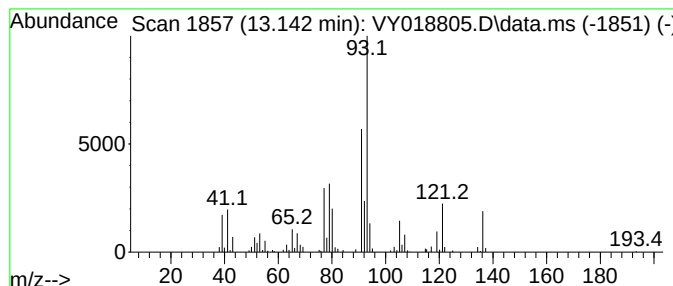
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070924S.M
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Peak Number 2 3-Carene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.142	20.68 ug/l	107292	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Carene	136	C10H16	013466-78-9	97
2			(+)-3-Carene	136	C10H16	000498-15-7	94
3			4-Carene, (1S,3R,6R)-(-)-	136	C10H16	005208-49-1	93
4			Cyclopentene, 3-isopropenyl-5,5-...	136	C10H16	1000162-25-4	90
5			Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	87



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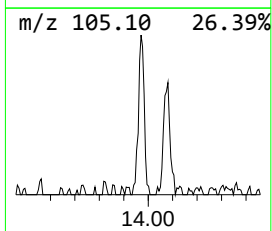
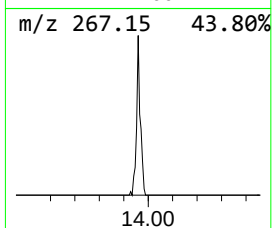
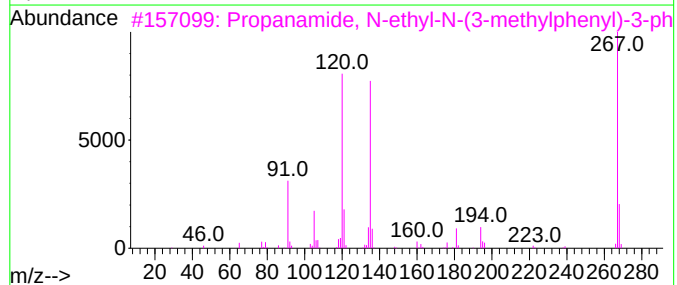
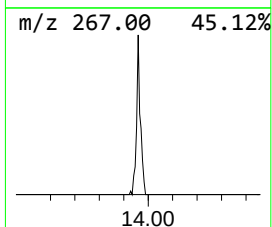
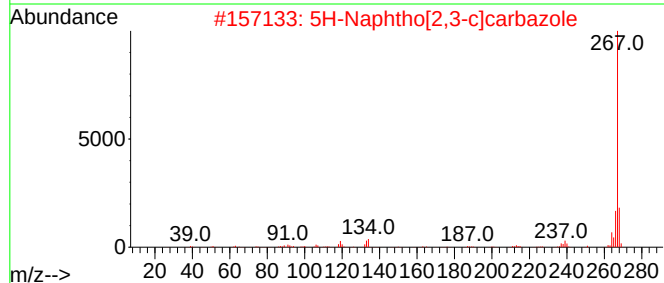
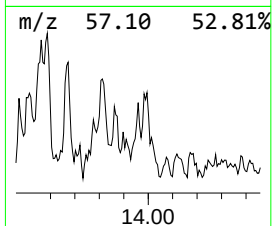
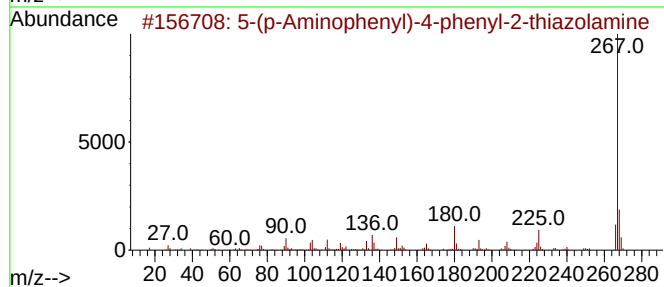
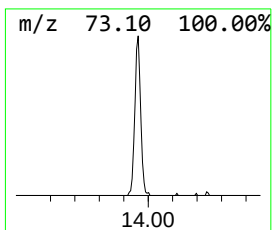
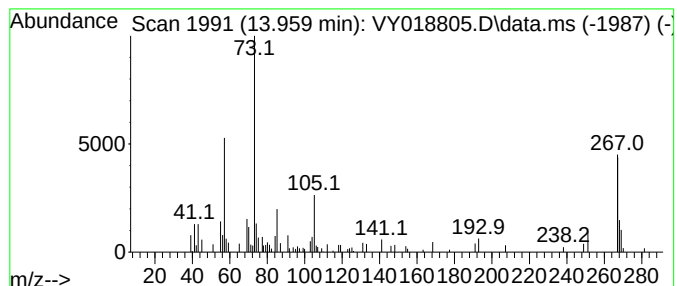
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070924S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown13.959 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.959	12.61 ug/l	65441	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-(p-Aminophenyl)-4-phenyl-2-thi...	267	C15H13N3S	092555-59-4	43
2			5H-Naphtho[2,3-c]carbazole	267	C20H13N	000198-96-9	43
3			Propanamide, N-ethyl-N-(3-methyl...	267	C18H21NO	1010308-21-3	43
4			13H-Dibenzo[a,i]carbazole	267	C20H13N	000239-64-5	43
5			4-(Methylamino)phenol, N,O-bis(t...	267	C13H25NOSi2	1000471-13-0	40



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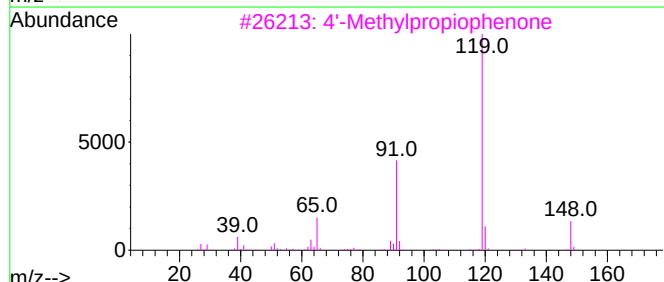
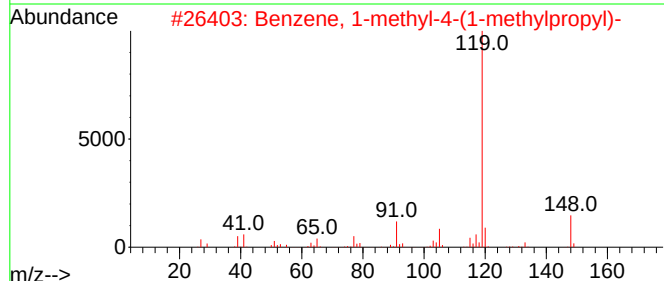
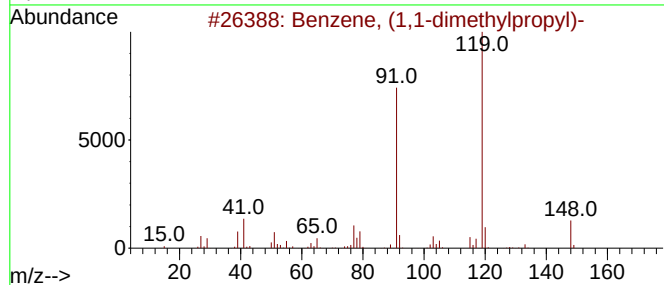
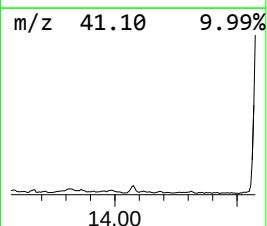
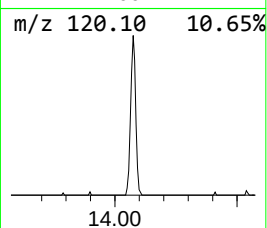
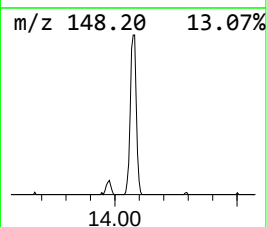
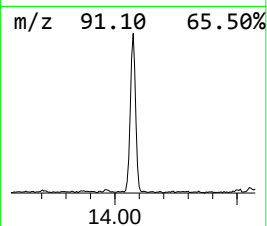
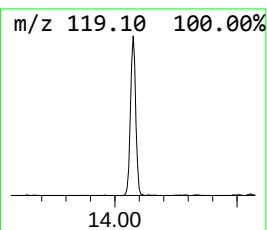
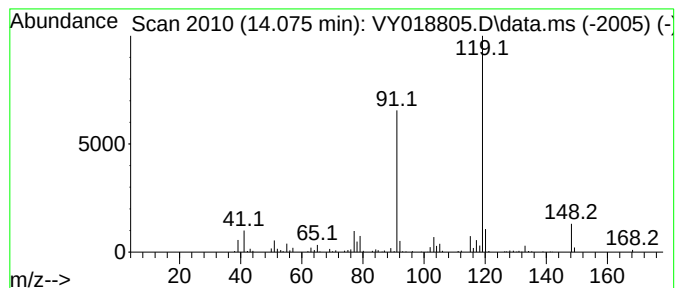
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Peak Number 4 Benzene, (1,1-dimethylpropyl)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.075	34.87 ug/l	180963	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	97
2			Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	87
3			4'-Methylpropiophenone	148	C10H12O	005337-93-9	80
4			Benzene, (1-ethylpropyl)-	148	C11H16	001196-58-3	80
5			Benzene, tert-butyl-	134	C10H14	000098-06-6	78



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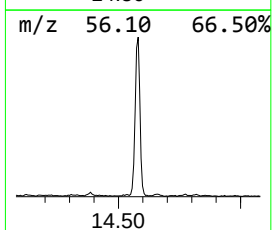
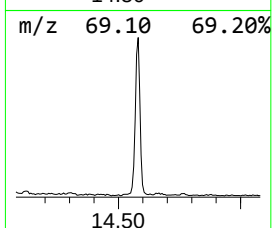
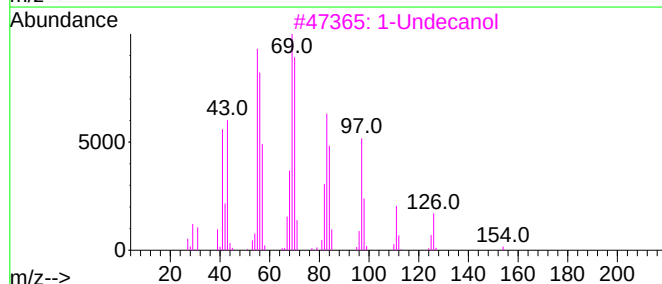
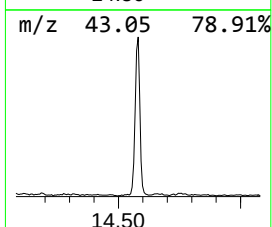
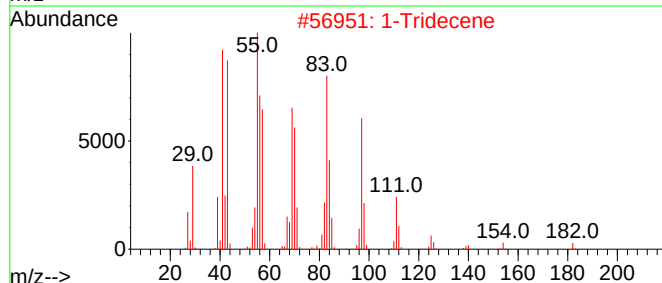
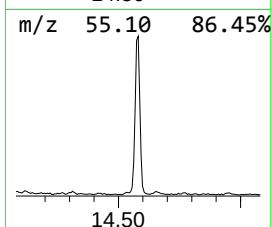
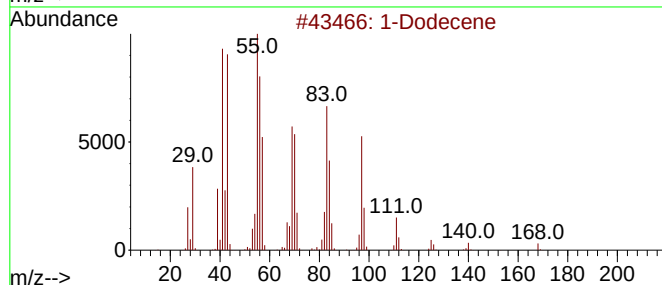
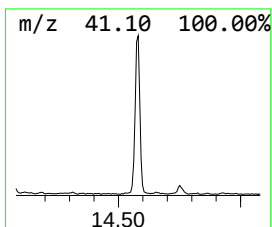
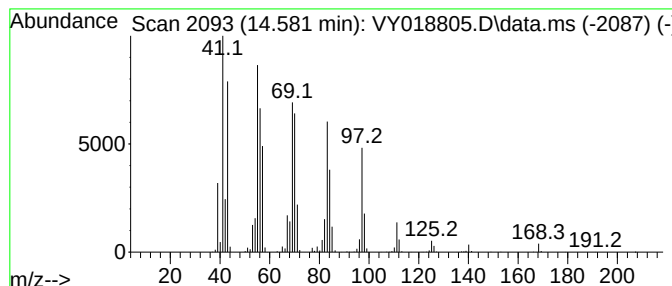
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Dodecene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.581	200.25 ug/l	1039080	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Dodecene	168	C12H24	000112-41-4	98
2			1-Tridecene	182	C13H26	002437-56-1	91
3			1-Undecanol	172	C11H24O	000112-42-5	87
4			Cetene	224	C16H32	000629-73-2	83
5			2-Nonanol, trifluoroacetate	240	C11H19F3O2	263911-21-3	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071224\
Data File : VY018805.D
Acq On : 12 Jul 2024 18:18
Operator : SY/MD
Sample : P3207-07
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RT-2929

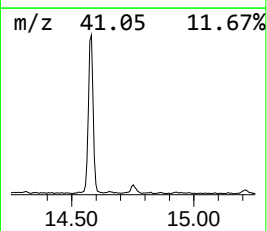
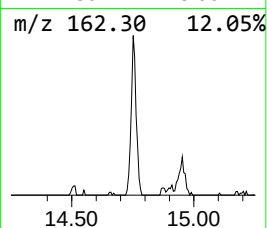
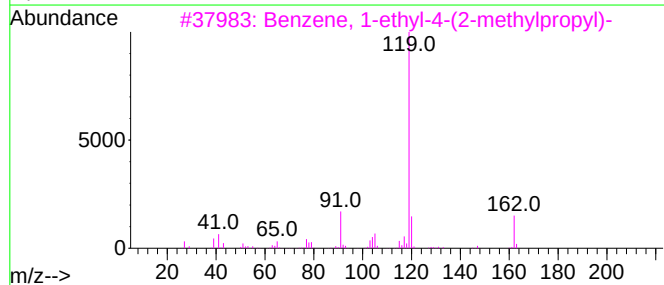
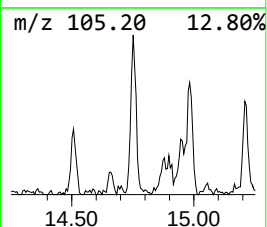
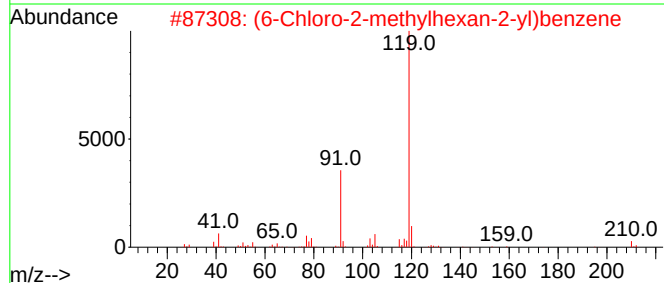
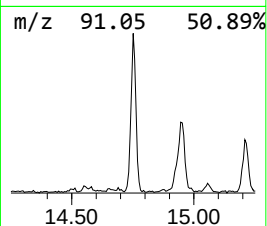
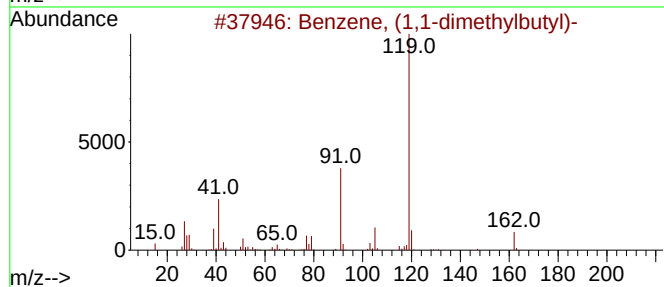
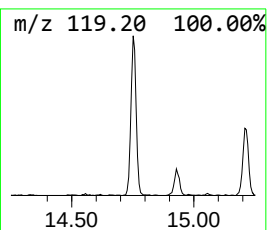
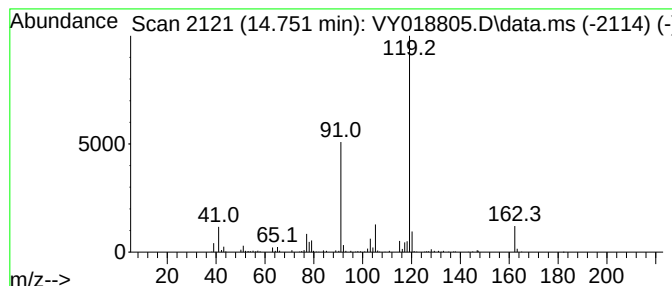
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, (1,1-dimethylbutyl)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.751	32.42 ug/l	168203	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1,1-dimethylbutyl)-	162	C12H18	001985-57-5	91
2			(6-Chloro-2-methylhexan-2-yl)ben...	210	C13H19Cl	1417621-45-4	86
3			Benzene, 1-ethyl-4-(2-methylprop...	162	C12H18	100319-40-2	78
4			Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	72
5			Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071224\
Data File : VY018805.D
Acq On : 12 Jul 2024 18:18
Operator : SY/MD
Sample : P3207-07
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RT-2929

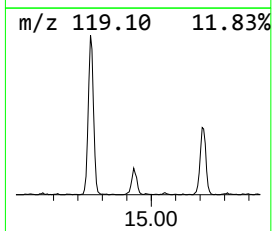
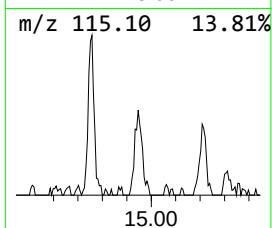
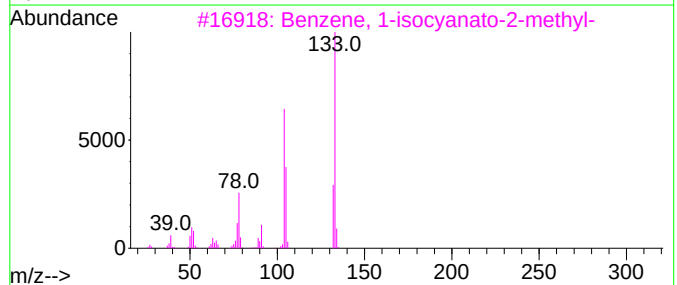
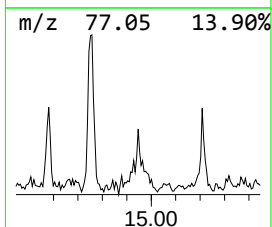
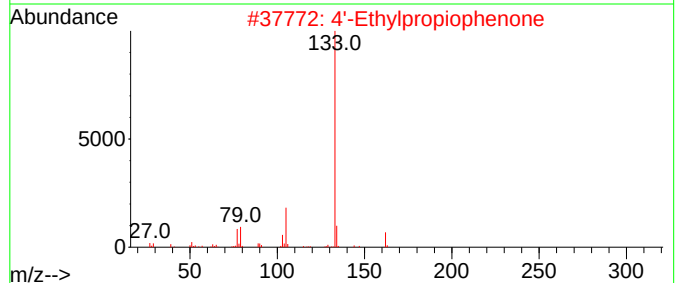
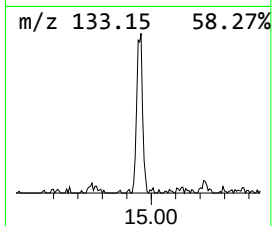
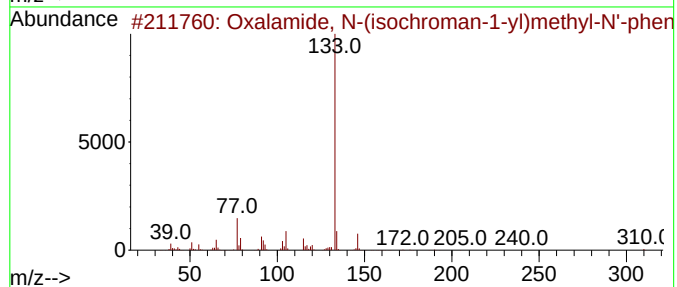
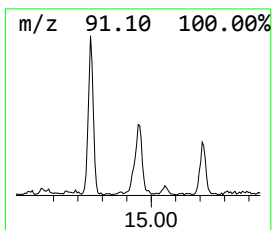
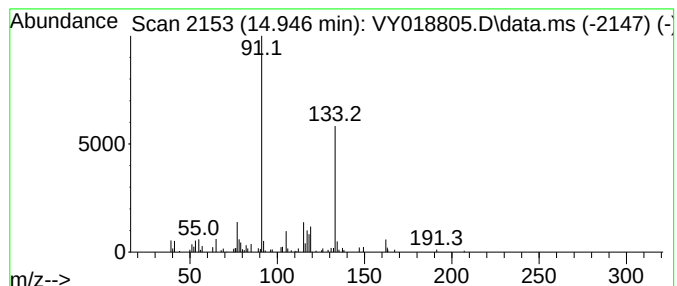
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Quant Title : SW846 8260

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

Peak Number 7 unknown14.946 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.946	10.53 ug/l	54639	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalamide, N-(isochroman-1-yl)me...	310	C18H18N2O3	1000304-26-0	43
2			4'-Ethylpropiophenone	162	C11H14O	027465-51-6	38
3			Benzene, 1-isocyanato-2-methyl-	133	C8H7NO	000614-68-6	38
4			2,3-Dihydroisoindol-1-one, 3-hyd...	253	C16H15NO2	1000303-19-2	38
5			Benzoxazole, 2-methyl-	133	C8H7NO	000095-21-6	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071224\
Data File : VY018805.D
Acq On : 12 Jul 2024 18:18
Operator : SY/MD
Sample : P3207-07
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RT-2929

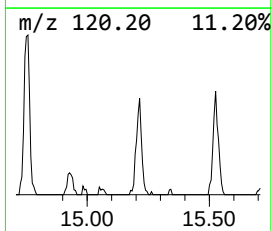
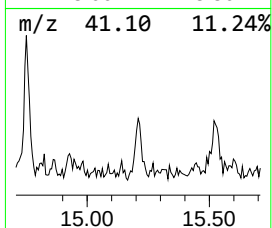
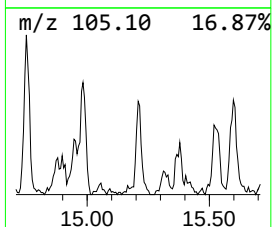
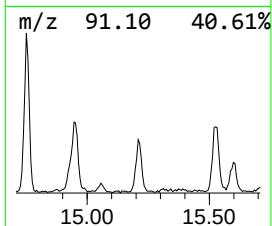
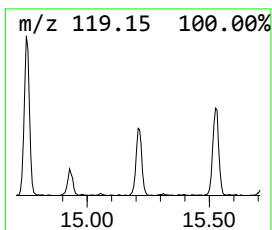
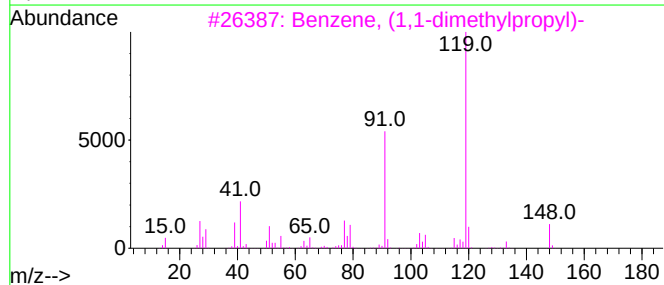
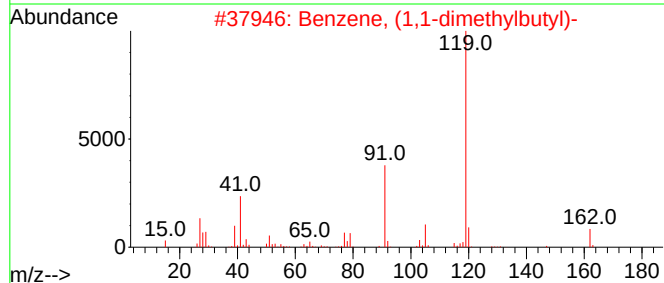
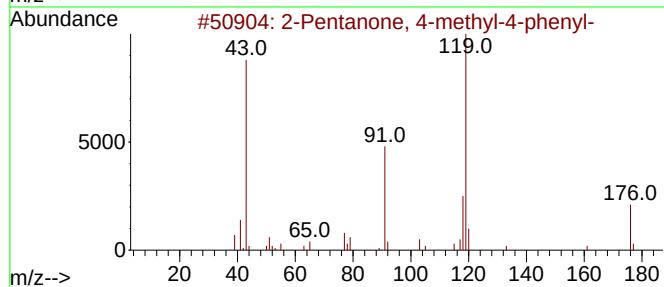
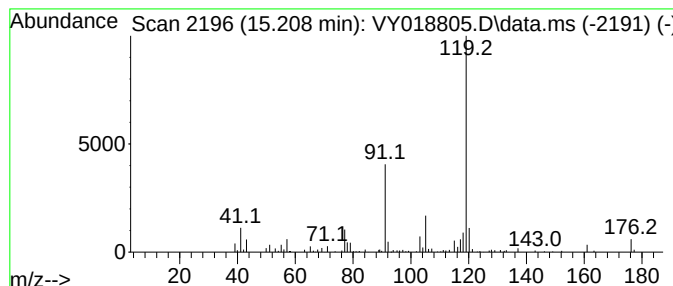
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Quant Title : SW846 8260

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

Peak Number 8 2-Pentanone, 4-methyl-4-phe... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.208	14.92 ug/l	77406	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methyl-4-phenyl-	176	C12H16O	007403-42-1	83
2			Benzene, (1,1-dimethylbutyl)-	162	C12H18	001985-57-5	78
3			Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	72
4			1,3,5-Cycloheptatriene, 3,7,7-tr...	134	C10H14	003479-89-8	72
5			Benzene, (1,1-dimethylnonyl)-	232	C17H28	055191-25-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071224\
Data File : VY018805.D
Acq On : 12 Jul 2024 18:18
Operator : SY/MD
Sample : P3207-07
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RT-2929

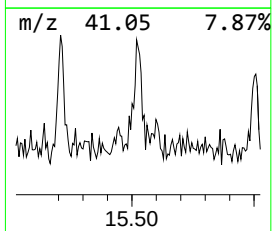
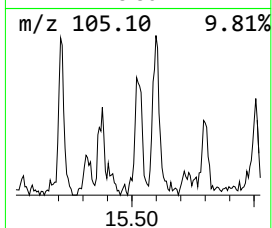
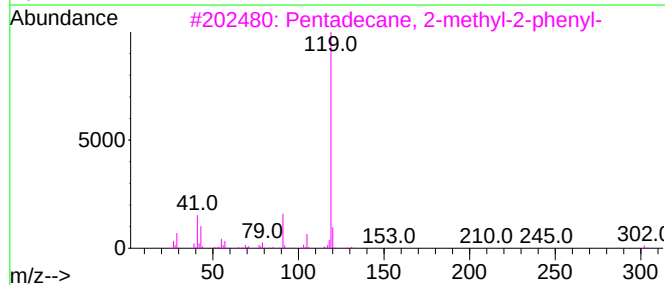
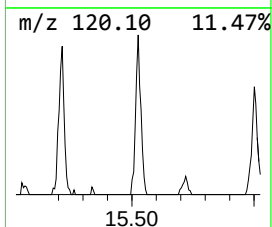
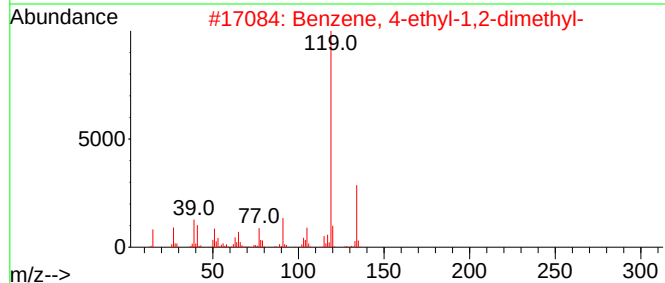
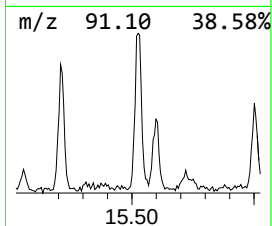
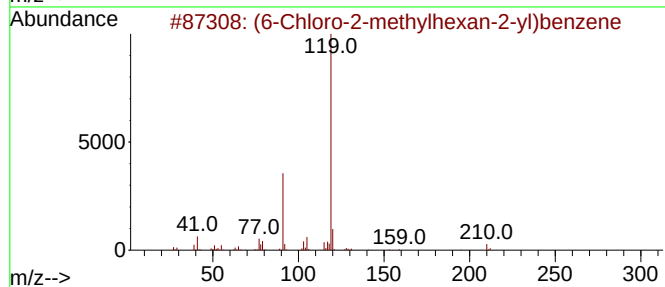
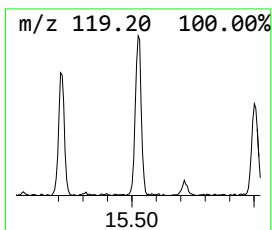
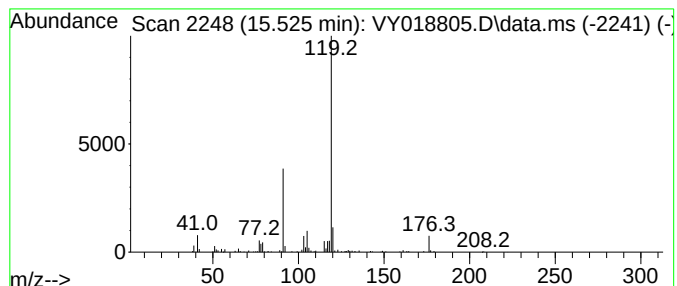
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Quant Title : SW846 8260

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

Peak Number 9 (6-Chloro-2-methylhexan-2-yl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.525	17.48 ug/l	90713	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(6-Chloro-2-methylhexan-2-yl)ben...	210	C13H19Cl	1417621-45-4	86
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	78
3			Pentadecane, 2-methyl-2-phenyl-	302	C22H38	029138-94-1	72
4			2,4,4,6-Tetramethyl-6-phenyl-1-h...	230	C17H26	1000293-27-9	72
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071224\
Data File : VY018805.D
Acq On : 12 Jul 2024 18:18
Operator : SY/MD
Sample : P3207-07
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RT-2929

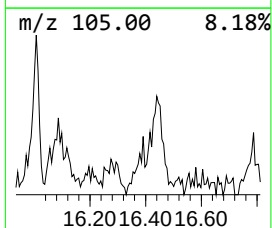
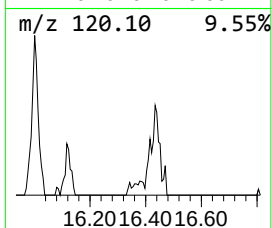
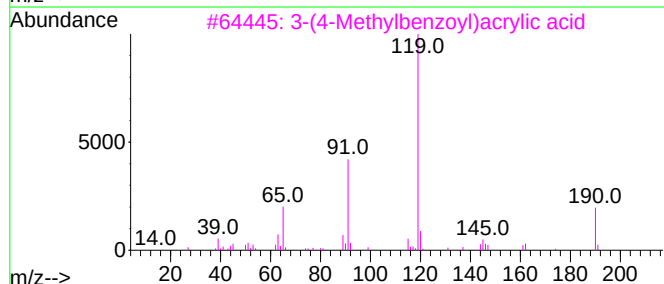
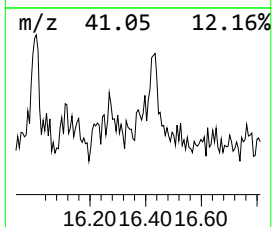
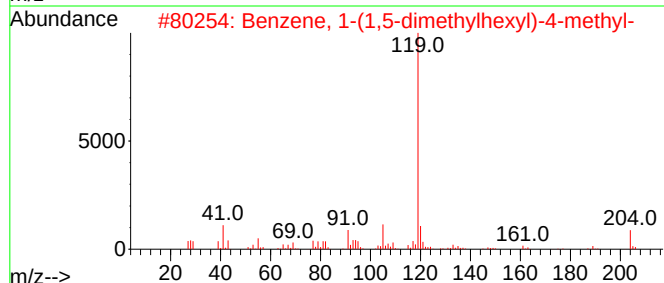
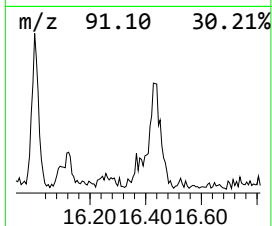
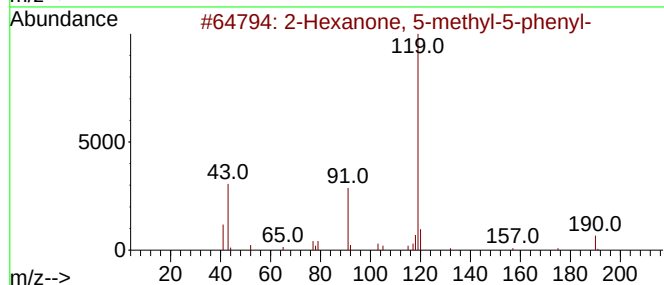
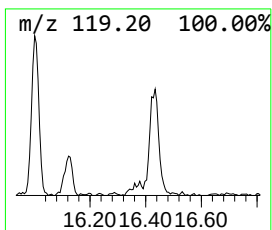
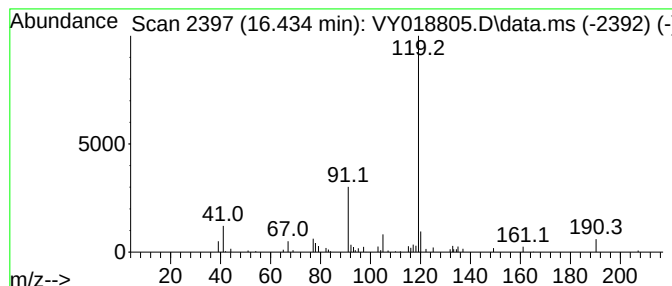
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Quant Title : SW846 8260

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

Peak Number 10 2-Hexanone, 5-methyl-5-phenyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.434	10.43 ug/l	54109	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanone, 5-methyl-5-phenyl-	190	C13H18O	014128-61-1	80		
2	Benzene, 1-(1,5-dimethylhexyl)-4...	204	C15H24	001461-02-5	78		
3	3-(4-Methylbenzoyl)acrylic acid	190	C11H10O3	020972-36-5	78		
4	Benzamide, 3-methyl-N-methyl-N-h...	373	C25H43NO	1000420-27-6	72		
5	Benzamide, 4-methyl-N-isobutyl-	191	C12H17NO	1000407-46-5	72		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071224\
Data File : VY018805.D
Acq On : 12 Jul 2024 18:18
Operator : SY/MD
Sample : P3207-07
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RT-2929

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070924S.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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3-Carene	13.142	20.7	ug/l	107292	4	13.422	259446	50.0
unknown13.959	13.959	12.6	ug/l	65441	4	13.422	259446	50.0
Benzene, (1,1-d...	14.075	34.9	ug/l	180963	4	13.422	259446	50.0
1-Dodecene	14.581	200.3	ug/l	1039080	4	13.422	259446	50.0
Benzene, (1,1-d...	14.751	32.4	ug/l	168203	4	13.422	259446	50.0
unknown14.946	14.946	10.5	ug/l	54639	4	13.422	259446	50.0
2-Pentanone, 4-...	15.208	14.9	ug/l	77406	4	13.422	259446	50.0
(6-Chloro-2-met...	15.525	17.5	ug/l	90713	4	13.422	259446	50.0
2-Hexanone, 5-m...	16.434	10.4	ug/l	54109	4	13.422	259446	50.0