

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY061625\
 Data File : VY022700.D
 Acq On : 16 Jun 2025 11:46
 Operator : SY/MD
 Sample : Q2322-01
 Misc : 5.01g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 CL-01-061325

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\82Y060225S.M
 Title : SW846 8260

Signal : TIC: VY022700.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.074	51	58	59	rBV4	7682	11553	5.46%	0.823%
2	2.178	73	75	77	rBV3	2226	2204	1.04%	0.157%
3	4.610	464	474	483	rBV5	3590	12108	5.72%	0.862%
4	5.641	635	643	652	rVB7	2375	6699	3.16%	0.477%
5	7.634	960	970	976	rBV	29242	70202	33.15%	4.999%
6	7.707	976	982	993	rVB	48906	112530	53.13%	8.013%
7	8.061	1033	1040	1052	rBV	28255	63754	30.10%	4.540%
8	8.616	1123	1131	1143	rBV	76272	160340	75.71%	11.417%
9	10.109	1369	1376	1385	rBV	121633	211783	100.00%	15.080%
10	10.432	1426	1429	1432	rVB4	2052	2119	1.00%	0.151%
11	11.414	1585	1590	1598	rBV	102125	177935	84.02%	12.670%
12	11.646	1612	1628	1629	rBV	22983	80125	37.83%	5.705%
13	11.975	1680	1682	1685	rBV4	3503	3187	1.50%	0.227%
14	12.408	1747	1753	1762	rVB	73750	123671	58.40%	8.806%
15	13.176	1875	1879	1891	rVB8	38433	127363	60.14%	9.069%
16	13.347	1901	1907	1913	rBV	91633	156666	73.97%	11.156%
17	14.029	2017	2019	2022	rBV4	4552	5662	2.67%	0.403%
18	14.060	2022	2024	2025	rBV2	5042	4044	1.91%	0.288%
19	15.139	2194	2201	2208	rBV2	7624	26868	12.69%	1.913%
20	15.291	2220	2226	2228	rBV6	17654	32392	15.29%	2.307%
21	16.035	2346	2348	2351	rBV4	2477	3257	1.54%	0.232%
22	16.352	2398	2400	2402	rBV3	2480	2145	1.01%	0.153%
23	16.383	2402	2405	2407	rBV4	1604	2126	1.00%	0.151%
24	16.529	2426	2429	2433	rVB5	2329	3489	1.65%	0.248%
25	16.657	2448	2450	2453	rBV3	1884	2139	1.01%	0.152%

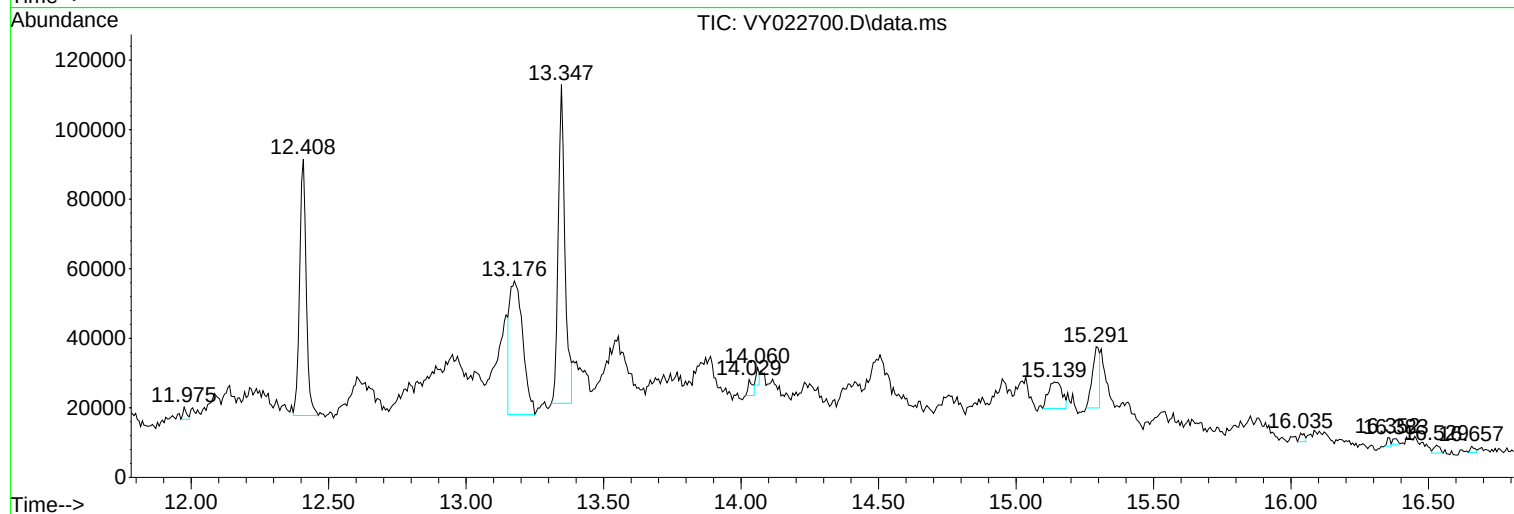
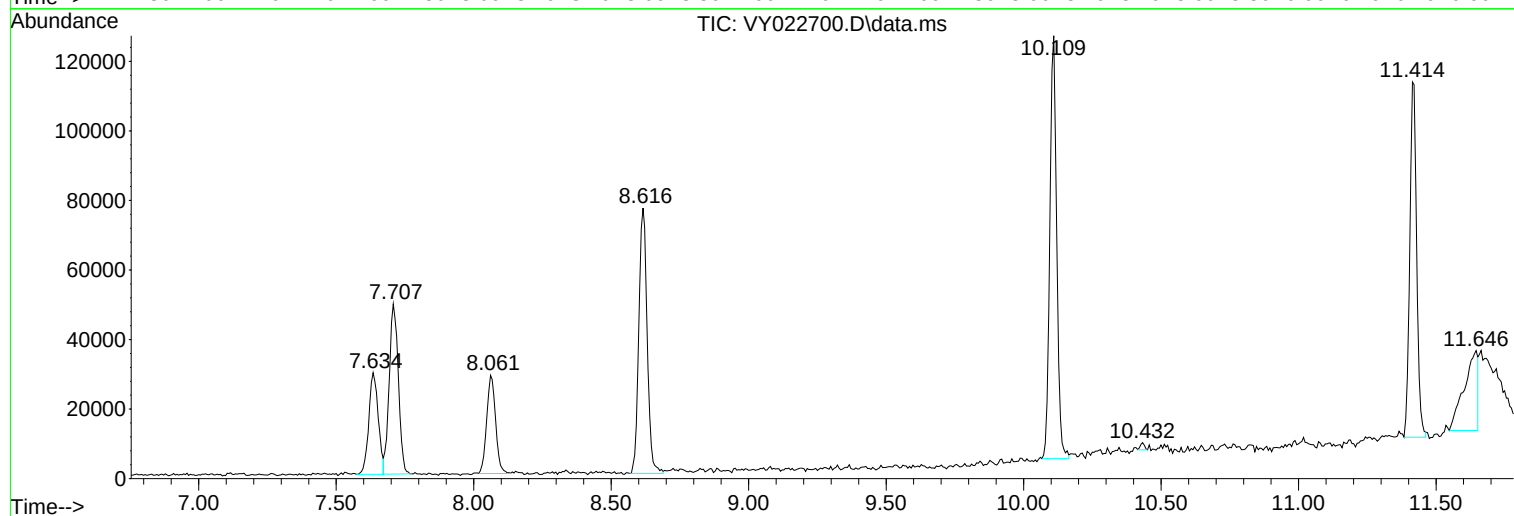
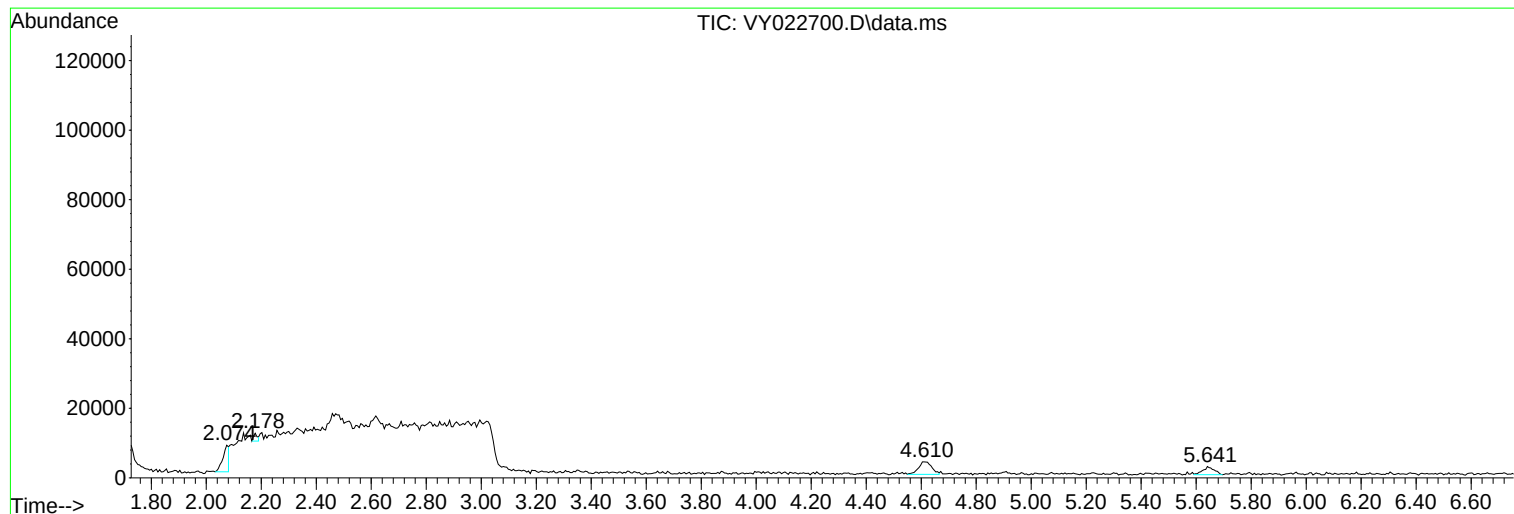
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CL-01-061325

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

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



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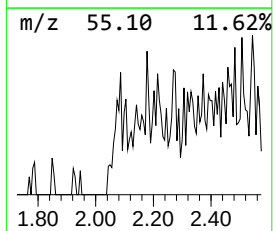
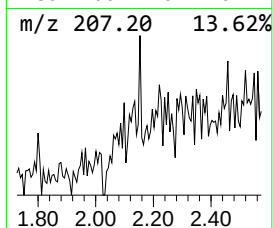
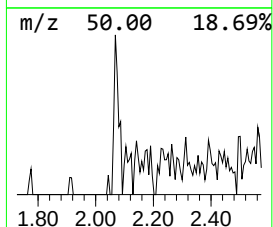
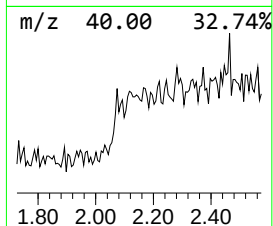
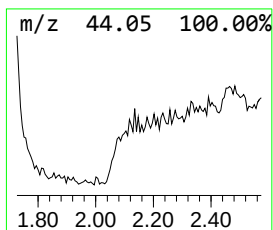
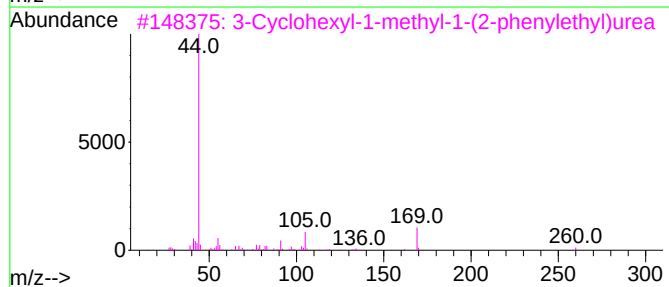
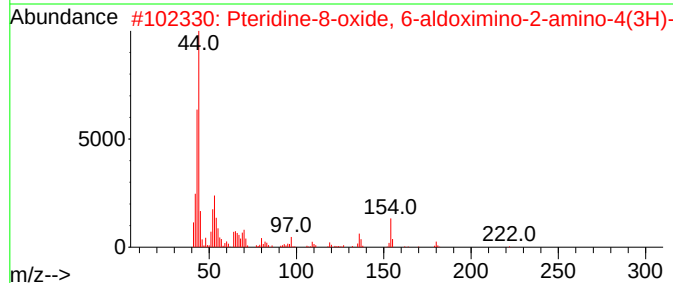
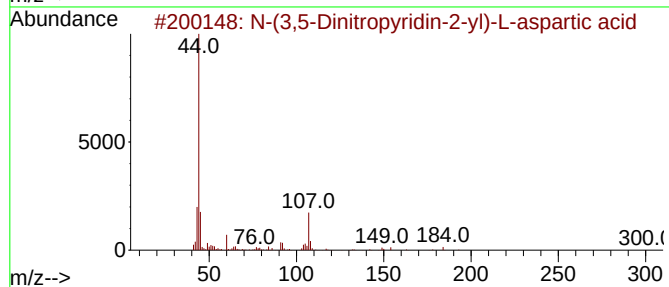
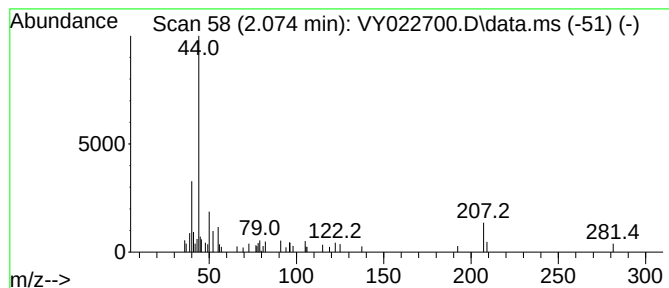
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.074 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.074	5.13 ug/l	11553	Pentafluorobenzene	7.707

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-(3,5-Dinitropyridin-2-yl)-L-as...	300	C9H8N4O8	035899-60-6	33
2			Pteridine-8-oxide, 6-aldoximino-...	222	C7H6N6O3	023663-23-2	9
3			3-Cyclohexyl-1-methyl-1-(2-pheny...	260	C16H24N2O	1024470-80-1	9
4			Atomoxetine	255	C17H21NO	083015-26-3	9
5			sec-Butylamine	73	C4H11N	013952-84-6	9



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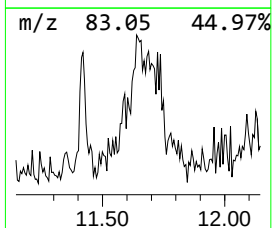
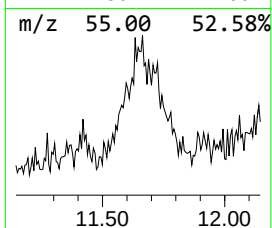
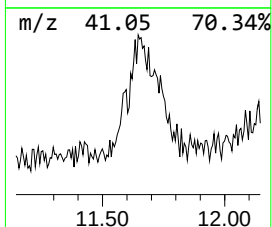
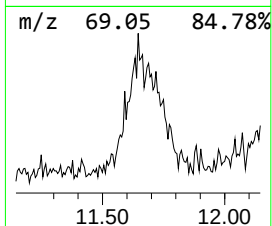
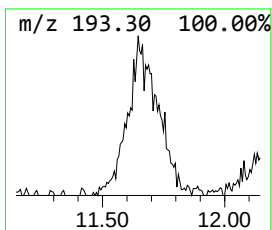
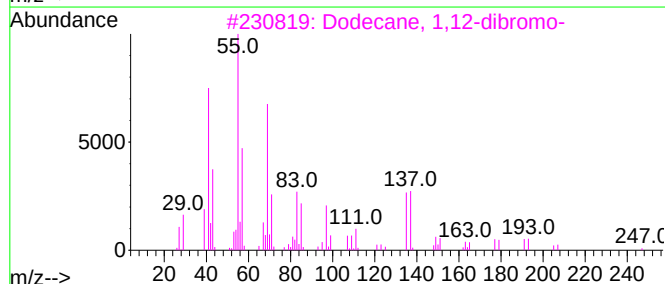
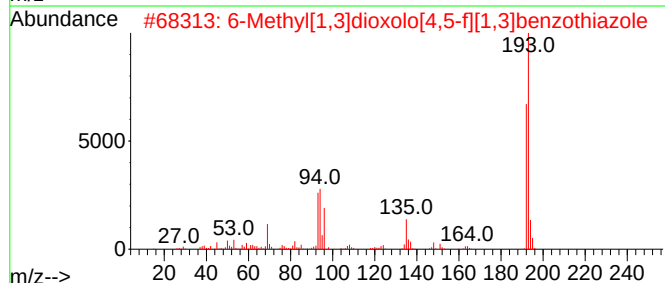
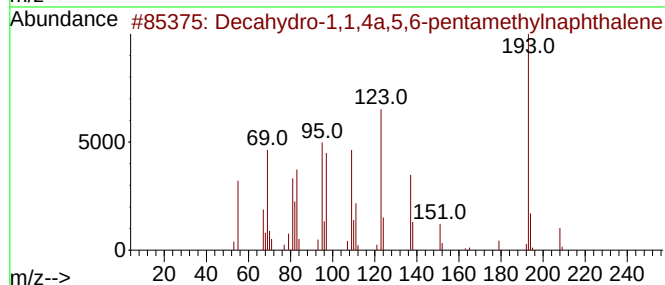
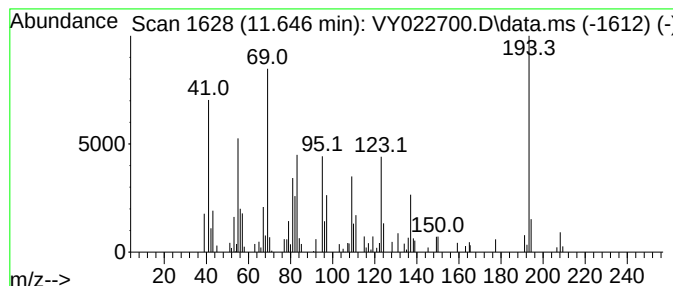
Instrument :
MSVOA_Y
ClientSampleId :
CL-01-061325

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

Peak Number 2 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.646	22.52 ug/l	80125	Chlorobenzene-d5	11.414	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	93
2	6-Methyl[1,3]dioxolo[4,5-f][1,3]...	193	C9H7NO2S	004791-94-0	35
3	Dodecane, 1,12-dibromo-	326	C12H24Br2	003344-70-5	27
4	benzoxazole, 5,6-dimethoxy-2-met...	193	C10H11NO3	1000395-98-9	18
5	2-Anthracenamine	193	C14H11N	000613-13-8	14



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Instrument :
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ClientSampleId :
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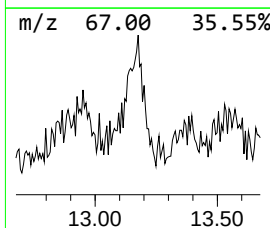
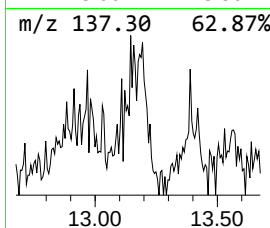
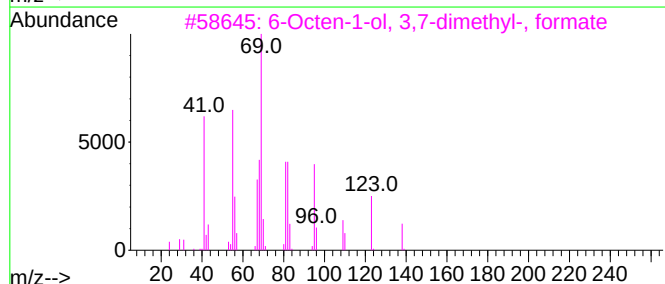
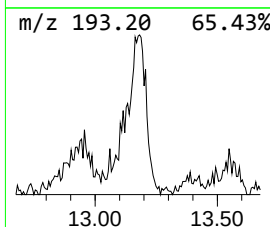
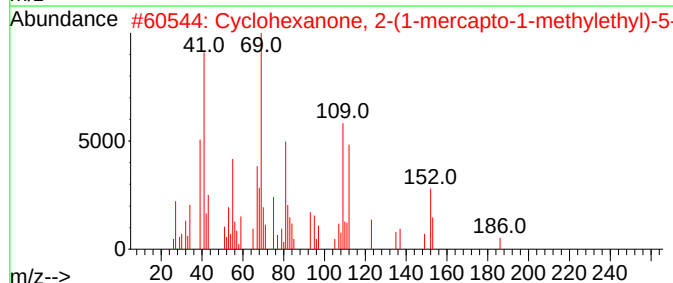
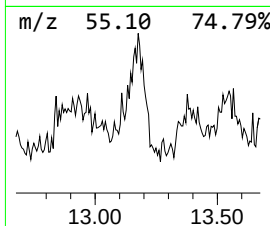
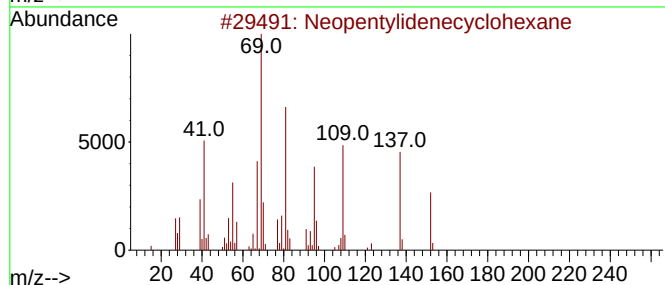
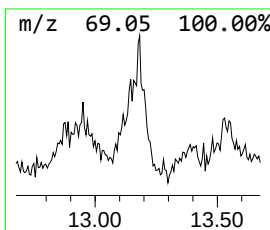
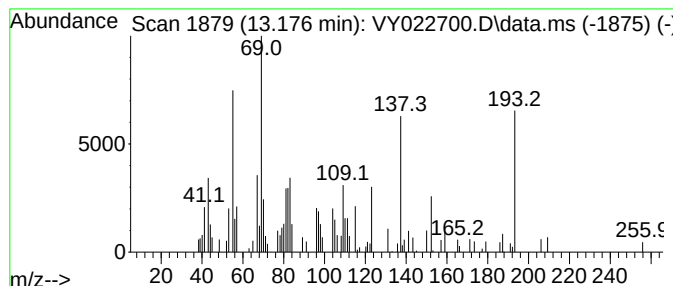
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown13.176 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.176	40.65 ug/l	127363	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Neopentylidenecyclohexane	152	C11H20	039546-80-0	37
2			Cyclohexanone, 2-(1-mercapto-1-m...	186	C10H18OS	033281-91-3	30
3			6-Octen-1-ol, 3,7-dimethyl-, for...	184	C11H20O2	000105-85-1	27
4			1-Bromo-8-chlorooctane	226	C8H16BrCl	1000438-83-6	25
5			3-Methyl-3-chloro-1-butene	104	C5H9Cl	002190-48-9	22



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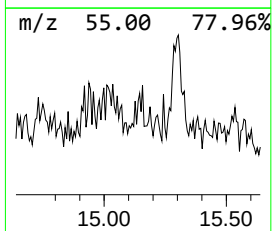
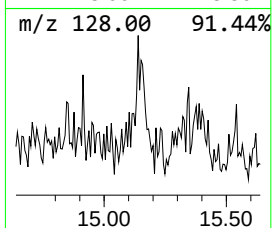
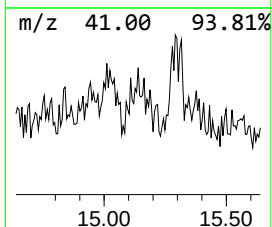
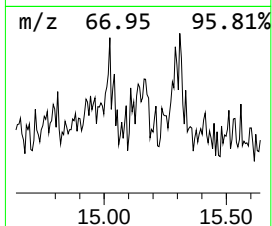
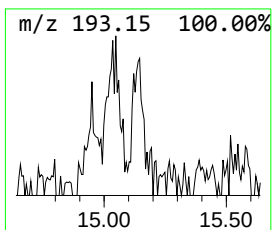
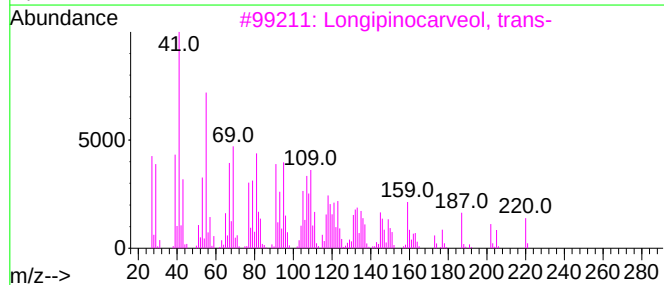
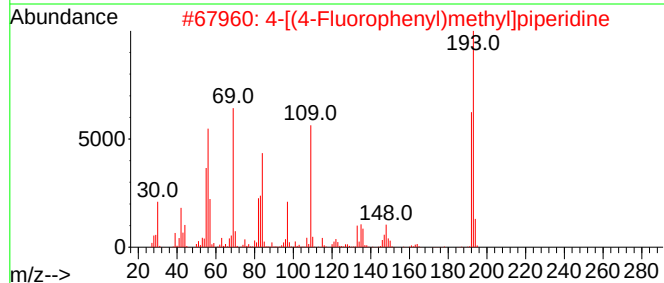
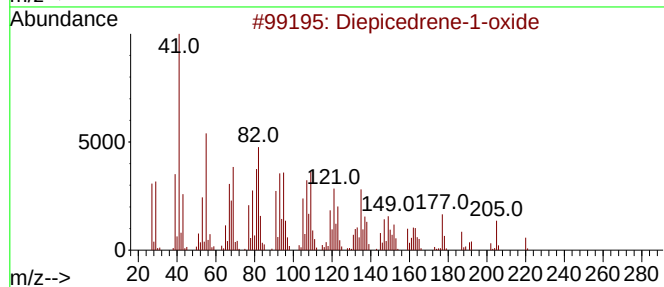
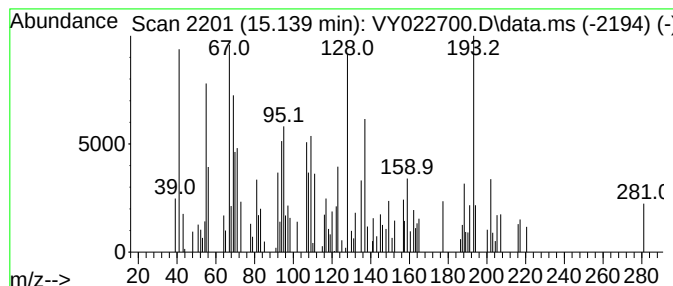
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Peak Number 4 unknown15.139 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.139	8.57 ug/l	26868	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diepicedrene-1-oxide	220	C15H24O	1000156-11-0	44
2			4-[(4-Fluorophenyl)methyl]piperi...	193	C12H16FN	092822-02-1	20
3			Longipinocarveol, trans-	220	C15H24O	1000159-36-5	18
4			1-Indolinecarboxaldehyde, 2-hydr...	193	C10H11NO3	013303-70-3	15
5			trans-Chrysanthenol	152	C10H16O	038043-83-3	11



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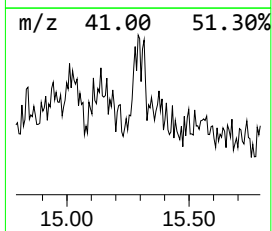
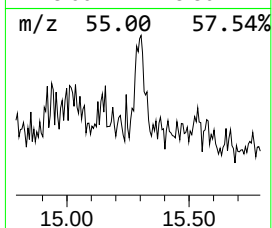
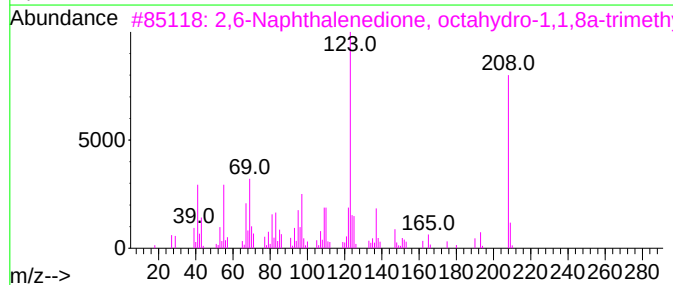
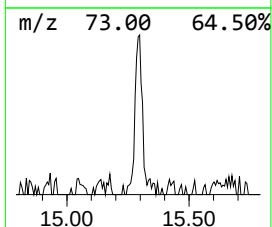
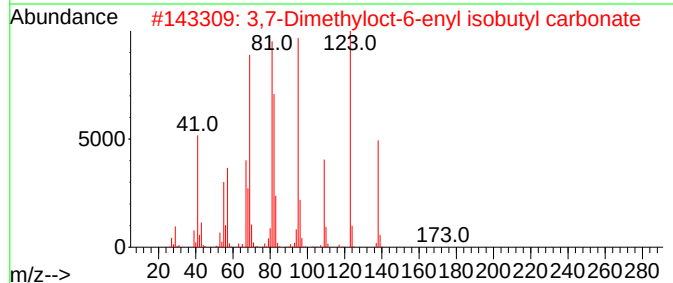
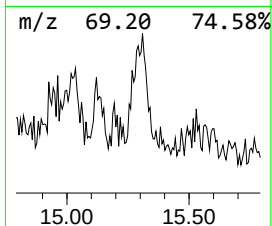
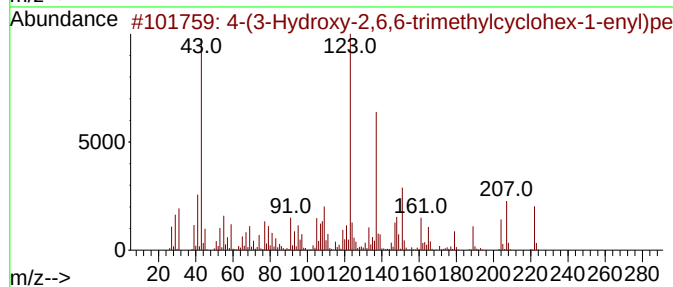
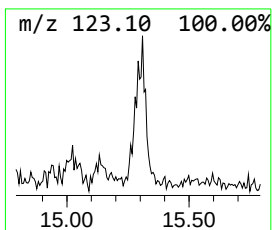
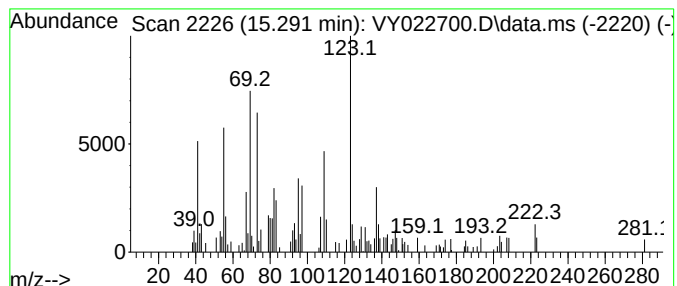
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 4-(3-Hydroxy-2,6,6-trimethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.291	10.34 ug/l	32392	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-(3-Hydroxy-2,6,6-trimethylcycl...	222	C14H22O2	097306-57-5	55
2			3,7-Dimethyloct-6-enyl isobutyl ...	256	C15H28O3	1000372-79-6	47
3			2,6-Naphthalenedione, octahydro-...	208	C13H20O2	057289-16-4	35
4			1,4-Hexadiene, 2,3,4,5-tetramethyl-	138	C10H18	051504-54-2	30
5			3-Fluorobenzoic acid, dodec-9-yn...	304	C19H25FO2	1000283-01-6	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.074	2.074	5.1	ug/l	11553	1	7.707	112530	50.0
Decahydro-1,1,4...	11.646	22.5	ug/l	80125	3	11.414	177935	50.0
unknown13.176	13.176	40.6	ug/l	127363	4	13.347	156666	50.0
unknown15.139	15.139	8.6	ug/l	26868	4	13.347	156666	50.0
4-(3-Hydroxy-2,...	15.291	10.3	ug/l	32392	4	13.347	156666	50.0