

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY101323\
 Data File : VY015957.D
 Acq On : 13 Oct 2023 15:07
 Operator : SY/MD
 Sample : 04844-05
 Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 OR-603-COMP-06

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\82Y101223S.M

Title : SW846 8260

Signal : TIC: VY015957.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.082	205	207	216	rVB3	960	1848	1.65%	0.323%
2	3.966	345	352	355	rBV2	952	2010	1.79%	0.352%
3	4.722	469	476	485	rVB3	3570	9843	8.77%	1.722%
4	5.765	638	647	653	rVB4	2025	4781	4.26%	0.837%
5	7.728	960	969	974	rBV2	11206	27108	24.15%	4.743%
6	7.795	974	980	989	rVB	16968	36885	32.86%	6.454%
7	8.149	1030	1038	1045	rBV3	13082	29227	26.04%	5.114%
8	8.697	1120	1128	1139	rVB	24375	49601	44.19%	8.679%
9	10.185	1365	1372	1379	rBV	38604	68526	61.04%	11.990%
10	10.343	1392	1398	1401	rBV	3075	5761	5.13%	1.008%
11	10.581	1432	1437	1445	rVB	7459	13048	11.62%	2.283%
12	11.331	1555	1560	1562	rBV5	1052	1607	1.43%	0.281%
13	11.495	1579	1587	1594	rBV	41077	67975	60.55%	11.894%
14	11.605	1599	1605	1607	rBV7	869	1384	1.23%	0.242%
15	12.154	1684	1695	1697	rBV7	3345	9922	8.84%	1.736%
16	12.489	1744	1750	1757	rBV3	45114	81460	72.57%	14.254%
17	13.428	1898	1904	1919	rVB	52602	112255	100.00%	19.642%
18	13.965	1987	1992	1998	rVB	21774	36222	32.27%	6.338%
19	15.318	2212	2214	2222	rVB8	7606	12040	10.73%	2.107%

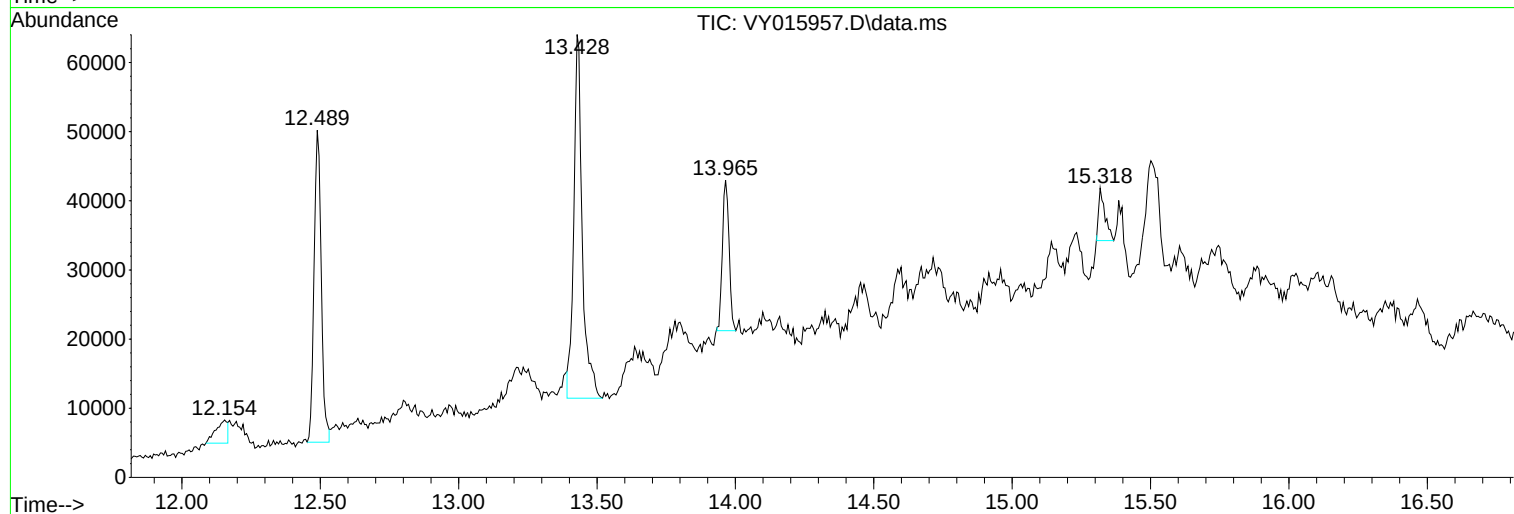
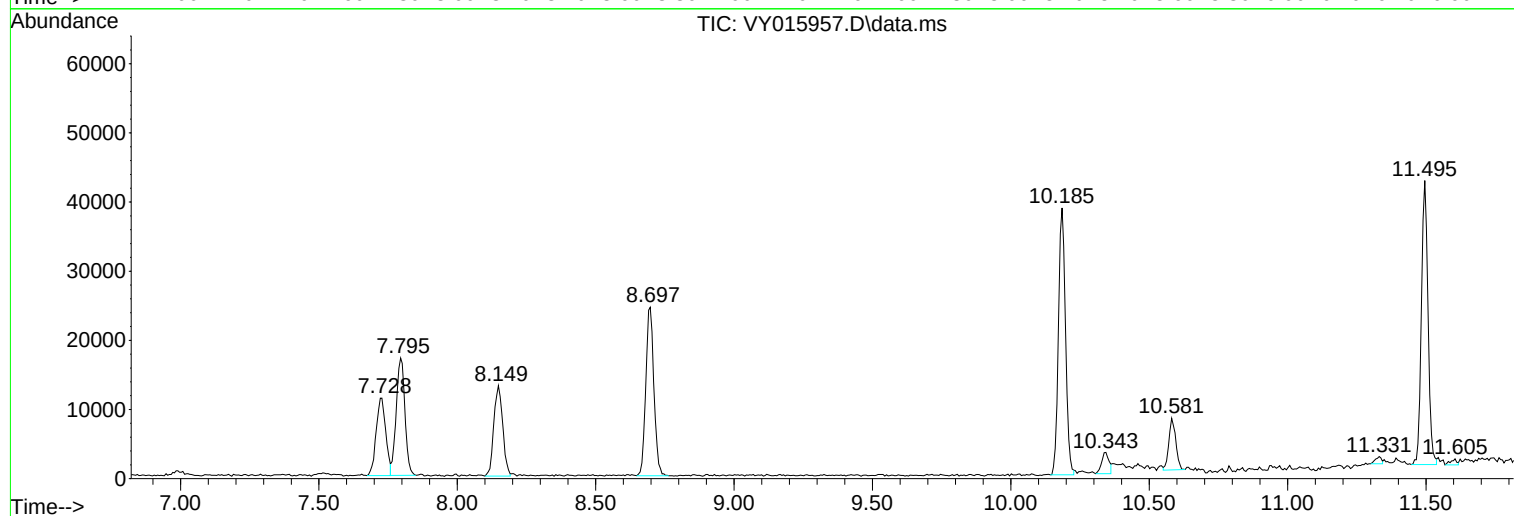
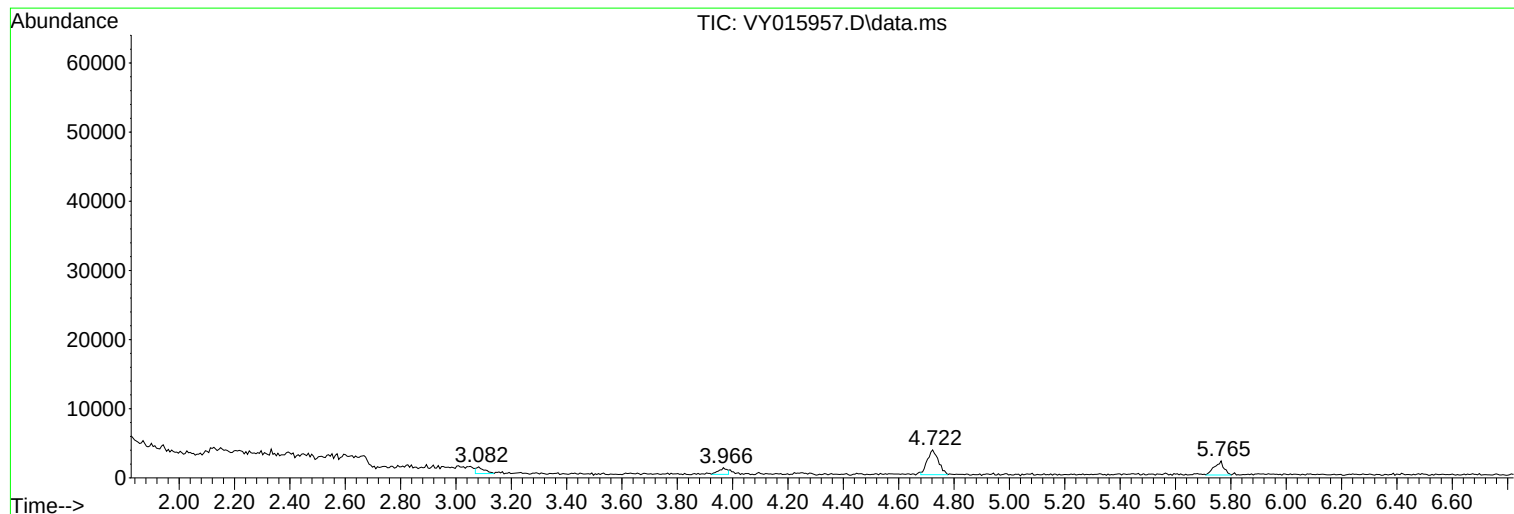
Sum of corrected areas: 571503

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TIC Integration Parameters: LSCINT.P



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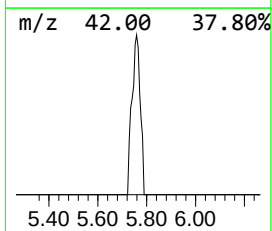
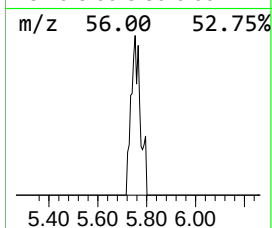
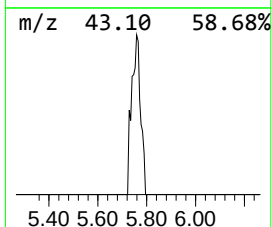
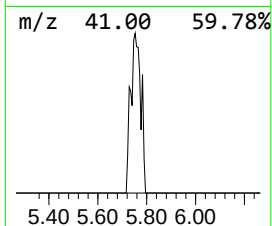
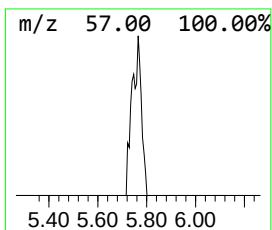
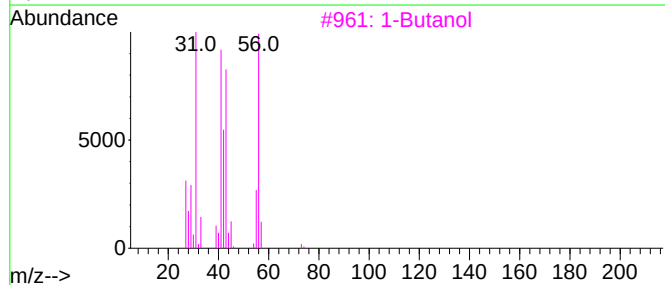
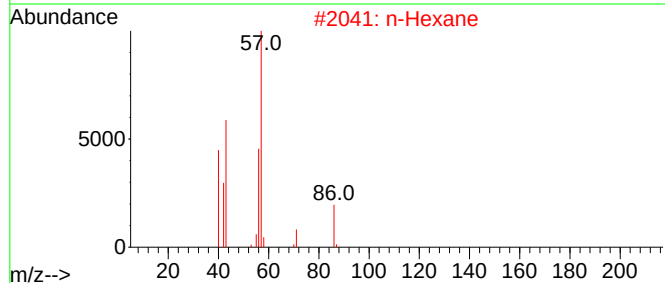
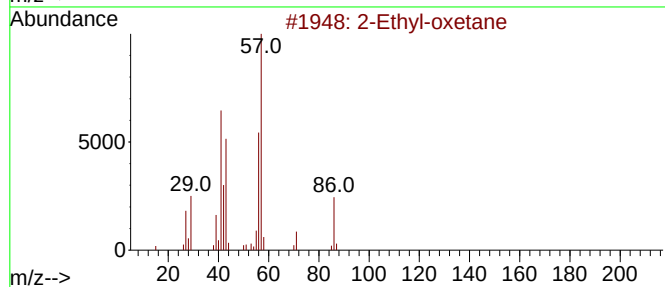
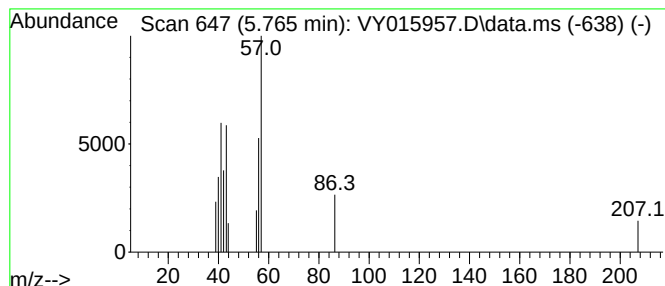
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y101223S.M
Quant Title : SW846 8260

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

Peak Number 1 2-Ethyl-oxetane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.765	6.48 ug/l	4781	Pentafluorobenzene	7.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	72
2			n-Hexane	86	C6H14	000110-54-3	64
3			1-Butanol	74	C4H10O	000071-36-3	28
4			Hydroperoxide, hexyl	118	C6H14O2	004312-76-9	25
5			Butyl aldoxime, 2-methyl-, syn-	101	C5H11NO	049805-56-3	9



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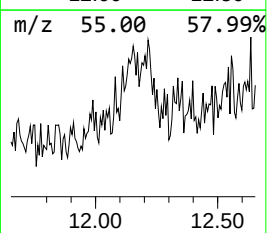
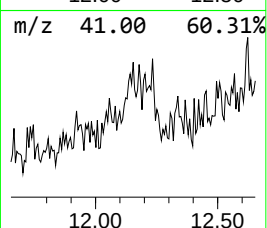
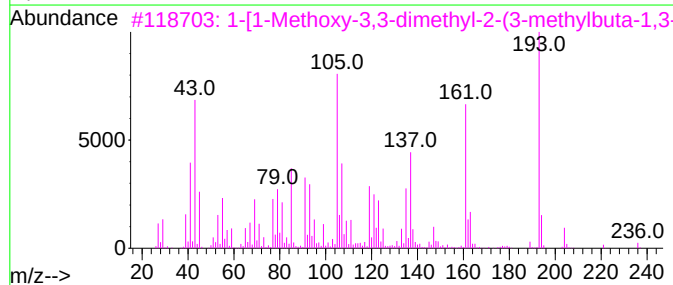
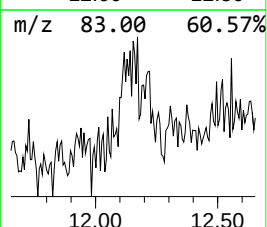
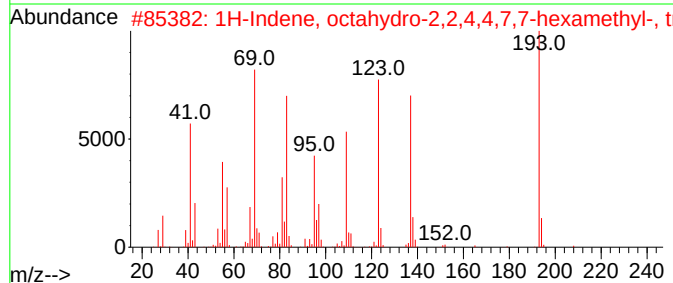
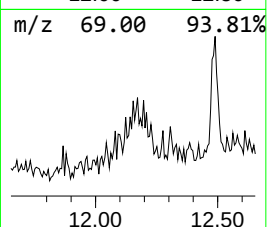
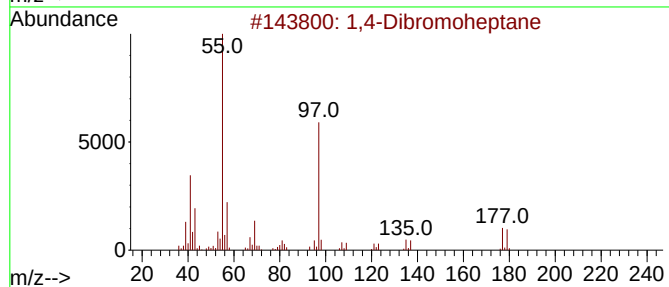
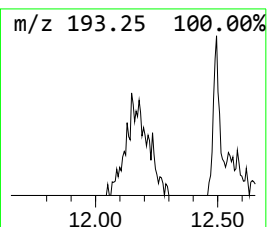
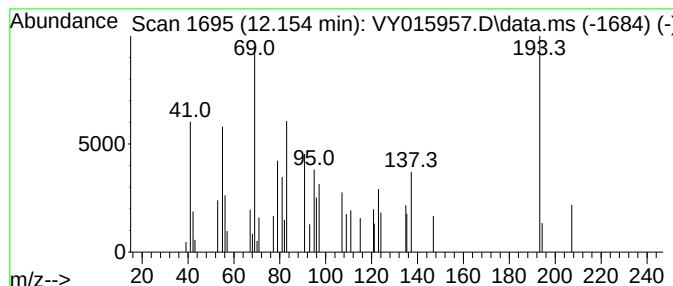
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y101223S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown12.154 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.154	7.30 ug/l	9922	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dibromoheptane	256	C7H14Br2	042474-23-7	47
2			1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	38
3			1-[1-Methoxy-3,3-dimethyl-2-(3-m...	236	C15H24O2	1000192-05-6	35
4			1-Bromo-8-chlorooctane	226	C8H16BrCl	1000438-83-6	35
5			Dodecane, 1,12-dibromo-	326	C12H24Br2	003344-70-5	32



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OR-603-COMP-06

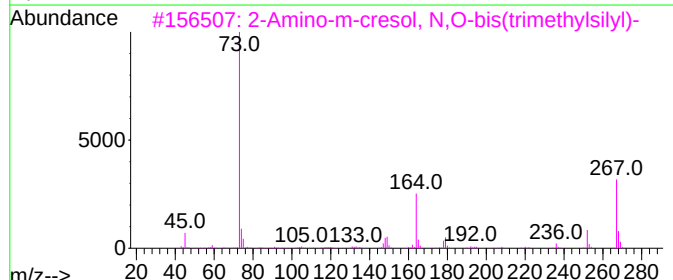
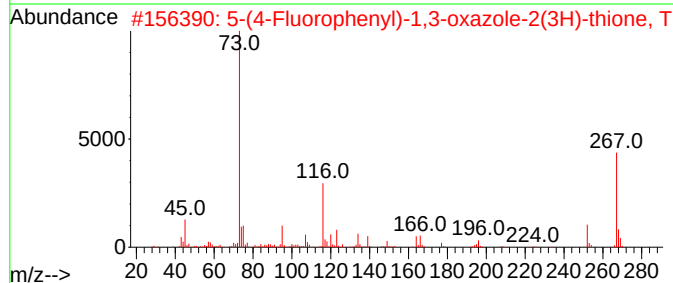
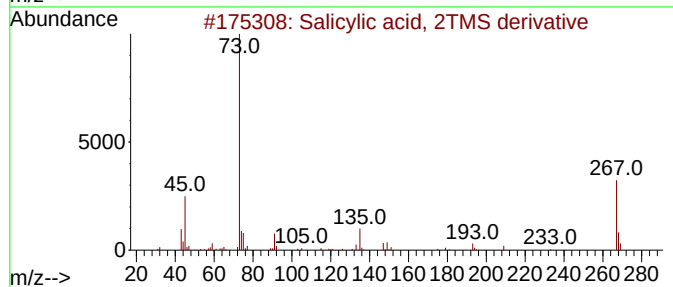
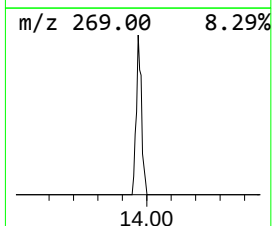
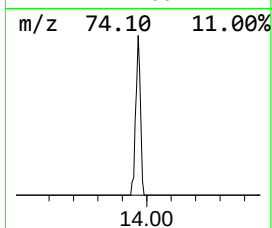
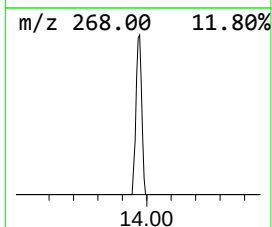
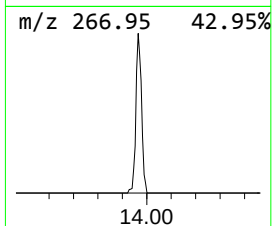
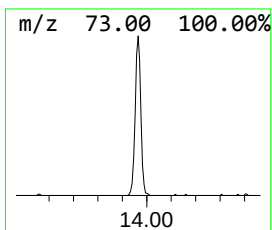
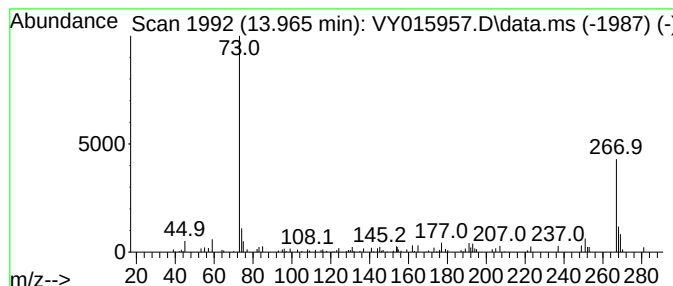
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Peak Number 4 Salicylic acid, 2TMS deriva... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.964	16.13 ug/l	36222	1,4-Dichlorobenzene-d4	13.434

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Salicylic acid, 2TMS derivative	282	C13H22O3Si2	003789-85-3	64
2			5-(4-Fluorophenyl)-1,3-oxazole-2...	267	C12H14FNOSSi	1000497-07-6	64
3			2-Amino-m-cresol, N,O-bis(trimet...	267	C13H25NOSi2	1000449-77-1	59
4			Acridone, TMS derivative	267	C16H17NOSi	1000478-16-0	45
5			2-[(Trimethylsilyl)oxy]-2-{4-[(t...	297	C14H27NO2Si2	1000473-27-9	42



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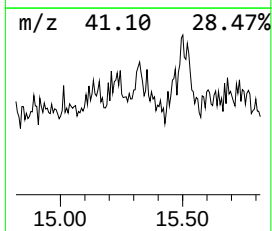
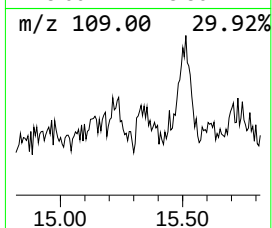
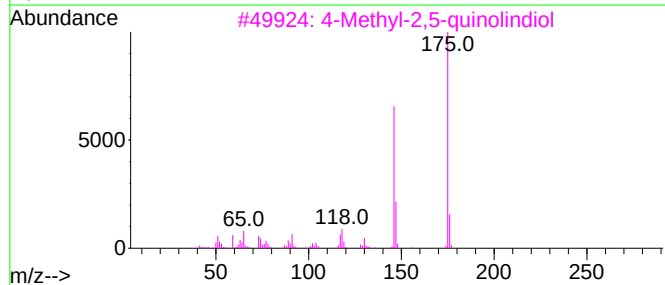
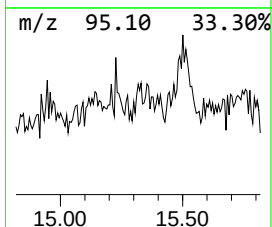
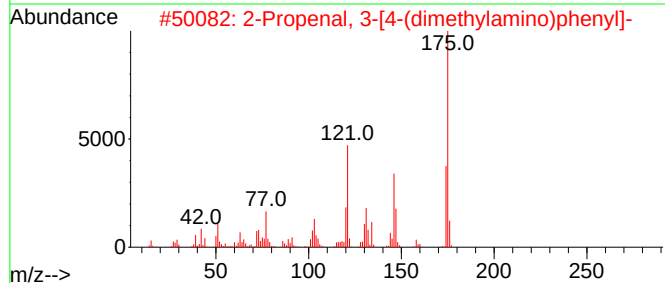
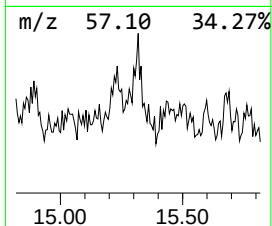
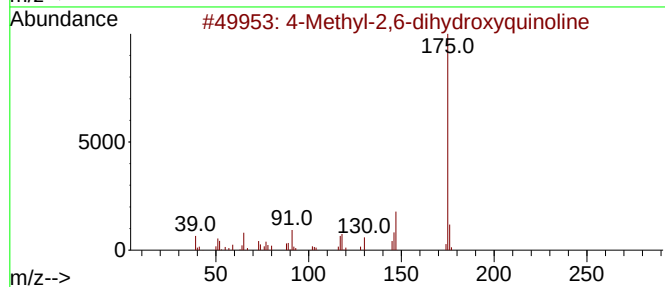
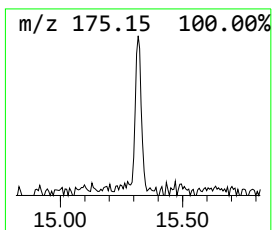
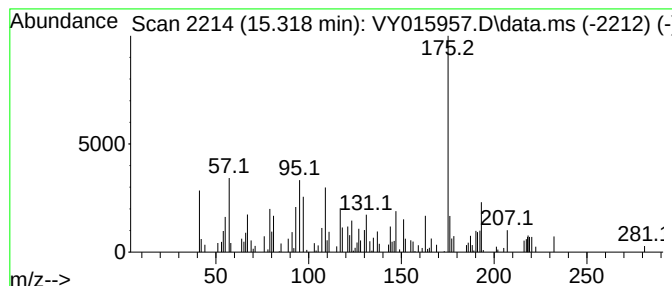
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Peak Number 5 unknown15.318 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.318	5.36 ug/l	12040	1,4-Dichlorobenzene-d4	13.434

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Methyl-2,6-dihydroxyquinoline	175	C10H9NO2	034982-01-9	30
2			2-Propenal, 3-[4-(dimethylamino)...]	175	C11H13NO	006203-18-5	30
3			4-Methyl-2,5-quinolindiol	175	C10H9NO2	131195-67-0	27
4			Benzene, 1,3-bis(1,1-dimethyleth...]	190	C14H22	001014-60-4	27
5			3,4-Dihydro-4-imino-3-methoxyqui...	175	C9H9N3O	015018-64-1	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Ethyl-oxetane	5.765	6.5	ug/l	4781	1	7.795	36885	50.0
unknown12.154	12.154	7.3	ug/l	9922	3	11.496	67975	50.0
Salicylic acid,...	13.964	16.1	ug/l	36222	4	13.434	112255	50.0
unknown15.318	15.318	5.4	ug/l	12040	4	13.434	112255	50.0