

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071524\
 Data File : VY018817.D
 Acq On : 15 Jul 2024 17:00
 Operator : SY/MD
 Sample : P3207-01
 Misc : 5.08g/5.0mL/MSVOA_Y/SOIL/B
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 CHRT-26899RE

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: VY018817.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.686	460	470	480	rBV2	13788	39183	7.02%	1.047%
2	4.948	502	513	518	rBV4	4441	14212	2.55%	0.380%
3	5.716	635	639	650	rVB4	2907	8172	1.46%	0.218%
4	7.704	956	965	971	rBV	86072	204689	36.69%	5.471%
5	7.777	971	977	993	rVB	142206	314883	56.45%	8.416%
6	8.130	1025	1035	1045	rBV	73749	162695	29.17%	4.348%
7	8.679	1116	1125	1139	rBV	217837	424633	76.12%	11.349%
8	10.173	1362	1370	1378	rBV	330958	557818	100.00%	14.909%
9	10.715	1454	1459	1463	rVB3	5132	7484	1.34%	0.200%
10	11.483	1577	1585	1594	rBV	311521	501323	89.87%	13.399%
11	12.331	1718	1724	1730	rVB5	10375	18745	3.36%	0.501%
12	12.477	1742	1748	1755	rBV	228594	359644	64.47%	9.612%
13	13.001	1828	1834	1841	rBV4	10353	18870	3.38%	0.504%
14	13.422	1897	1903	1911	rBV	259450	398113	71.37%	10.641%
15	13.641	1934	1939	1946	rVB10	4196	10682	1.91%	0.286%
16	13.739	1950	1955	1960	rBV6	9610	19170	3.44%	0.512%
17	13.855	1970	1974	1981	rVB10	3927	9156	1.64%	0.245%
18	13.922	1981	1985	1987	rBV5	4009	5594	1.00%	0.150%
19	13.958	1987	1991	2000	rVB7	9852	19817	3.55%	0.530%
20	14.038	2000	2004	2007	rBV6	3321	5965	1.07%	0.159%
21	14.123	2013	2018	2021	rBV5	6929	11385	2.04%	0.304%
22	14.251	2035	2039	2041	rBV2	12815	18461	3.31%	0.493%
23	14.288	2041	2045	2050	rVV4	17454	34413	6.17%	0.920%
24	14.330	2050	2052	2056	rVB	6191	8101	1.45%	0.217%
25	14.391	2056	2062	2064	rBV5	13184	22800	4.09%	0.609%
26	14.416	2064	2066	2070	rVV5	13424	18415	3.30%	0.492%
27	14.477	2071	2076	2079	rVB7	6573	13156	2.36%	0.352%
28	14.617	2095	2099	2103	rBV7	6587	11541	2.07%	0.308%
29	14.672	2103	2108	2109	rBV5	10488	14903	2.67%	0.398%
30	14.733	2114	2118	2122	rVB7	11109	17932	3.21%	0.479%
31	14.788	2123	2127	2129	rBV4	6109	7227	1.30%	0.193%
32	14.873	2132	2141	2147	rBV8	25098	59332	10.64%	1.586%
33	14.940	2148	2152	2157	rVB3	23392	34943	6.26%	0.934%
34	15.001	2158	2162	2165	rBV	12998	20722	3.71%	0.554%
35	15.184	2190	2192	2197	rBV5	5965	6677	1.20%	0.178%
36	15.269	2202	2206	2210	rBV5	23983	47609	8.53%	1.272%

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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

37	16.111	2340	2344	2349	rBV8	21561	47610	8.54%	1.272%
38	16.476	2400	2404	2410	rVB6	62161	114291	20.49%	3.055%
39	16.604	2420	2425	2439	rBV6	32962	131102	23.50%	3.504%

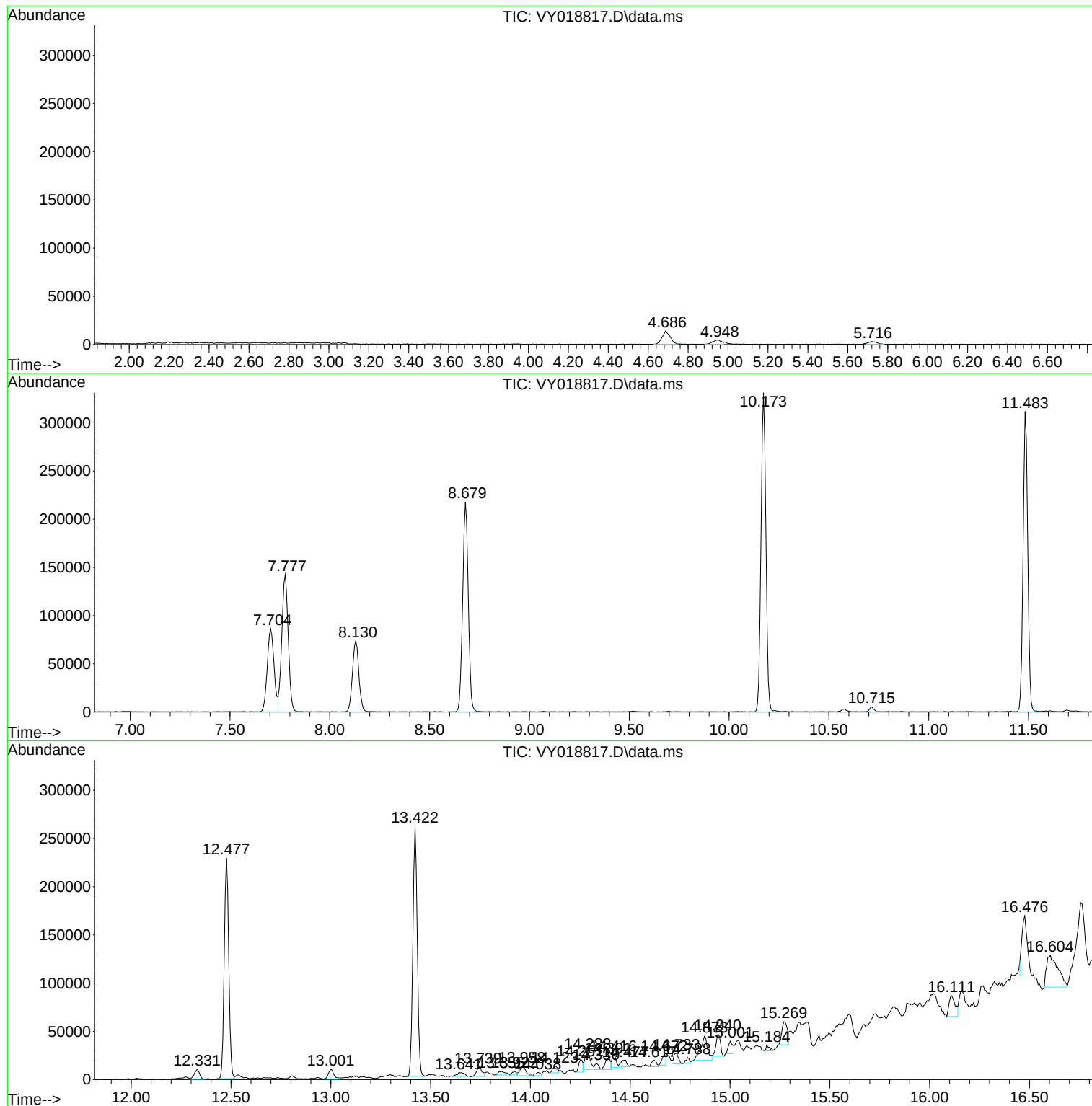
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070924S.M
Quant Title : SW846 8260

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



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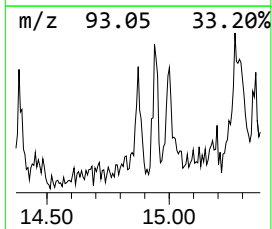
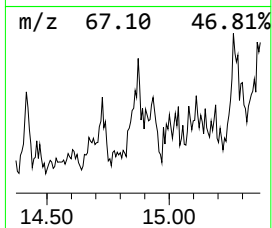
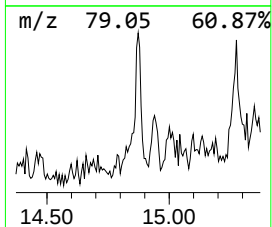
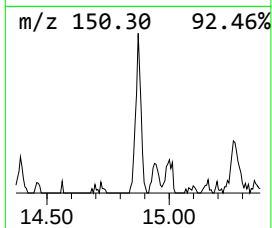
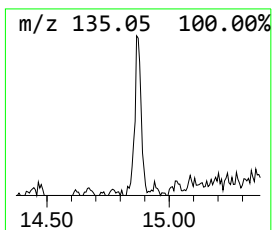
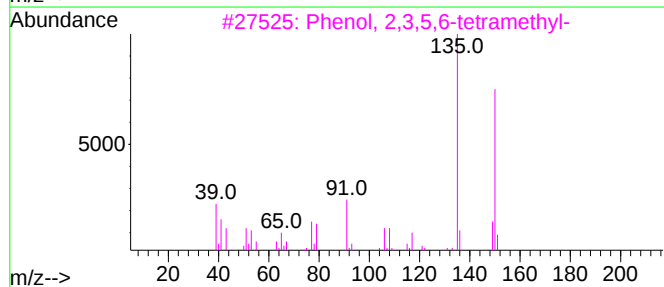
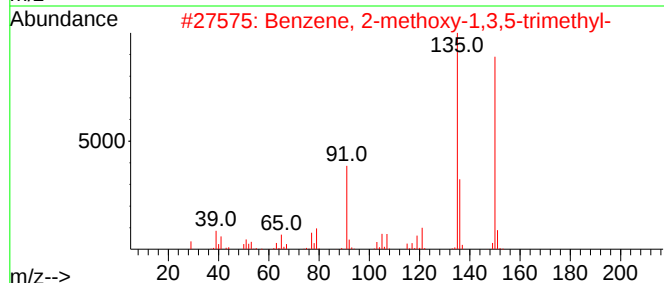
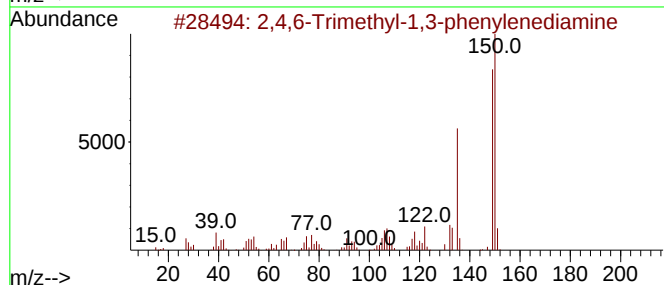
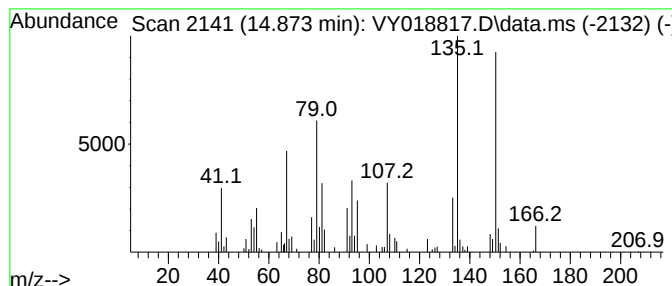
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070924S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown14.873 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.873	7.45 ug/l	59332	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,6-Trimethyl-1,3-phenylenedia...	150	C9H14N2	003102-70-3	49		
2	Benzene, 2-methoxy-1,3,5-trimethyl-	150	C10H14O	004028-66-4	43		
3	Phenol, 2,3,5,6-tetramethyl-	150	C10H14O	000527-35-5	43		
4	Ethyltetramethylcyclopentadiene	150	C11H18	057693-77-3	43		
5	Phenol, 2,3,4,6-tetramethyl-	150	C10H14O	003238-38-8	43		



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-26899RE

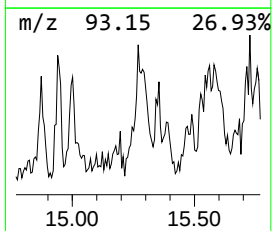
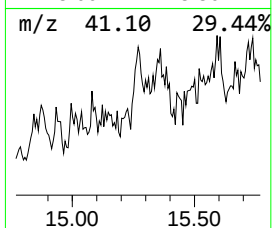
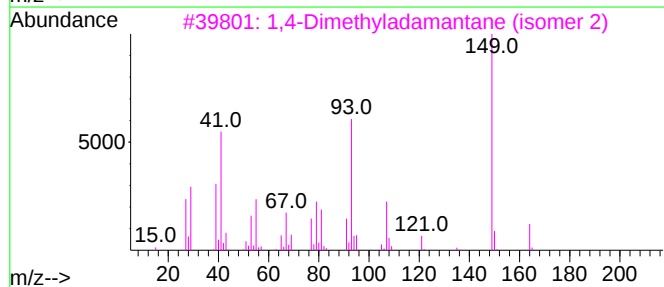
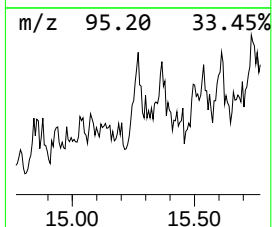
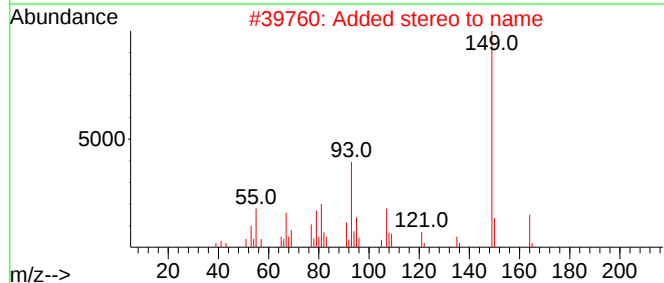
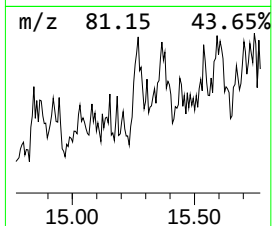
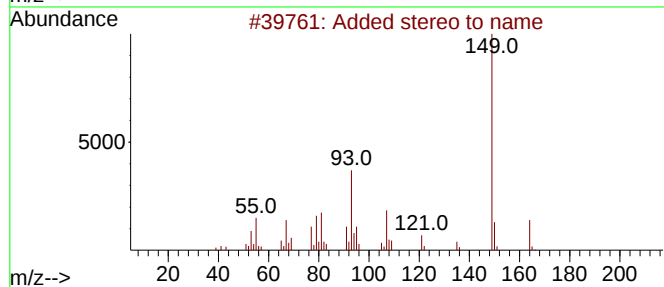
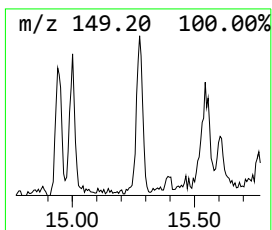
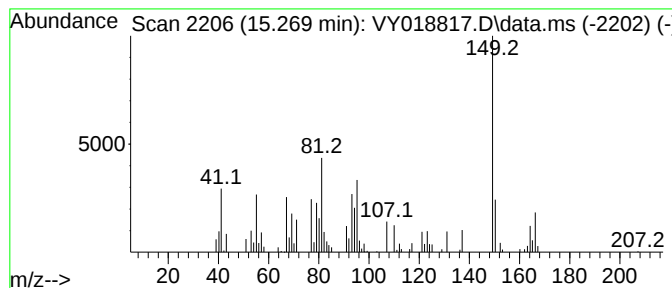
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070924S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown15.269 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.269	5.98 ug/l	47609	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Added stereo to name			164	C12H20	024145-89-9	49
2	Added stereo to name			164	C12H20	024145-88-8	49
3	1,4-Dimethyladamantane (isomer 2)			164	C12H20	1000460-67-1	43
4	Phthalic acid, 3-methyl-4-nitro...			357	C19H19NO6	1000382-59-8	40
5	Tricyclo[4.3.1.1(3,8)]undecane, ...			184	C11H17Cl	027011-46-7	38



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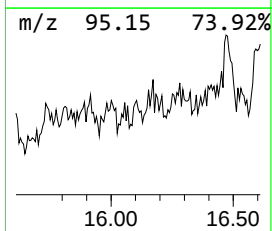
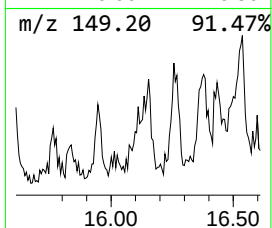
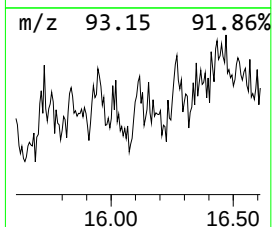
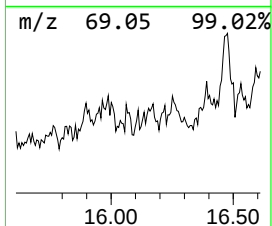
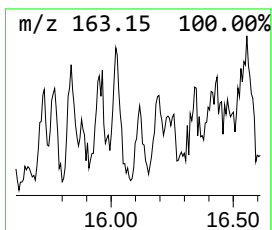
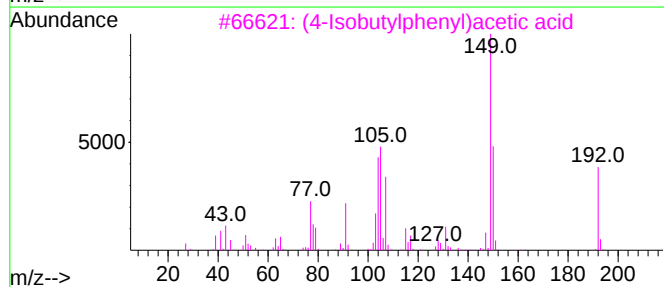
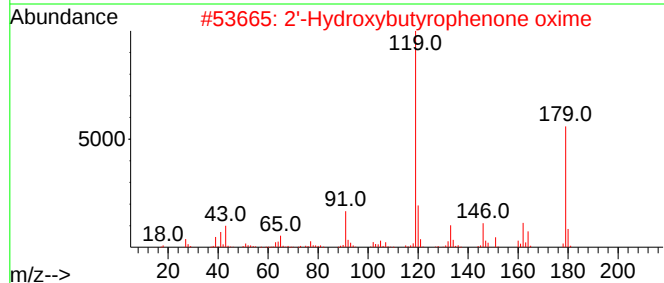
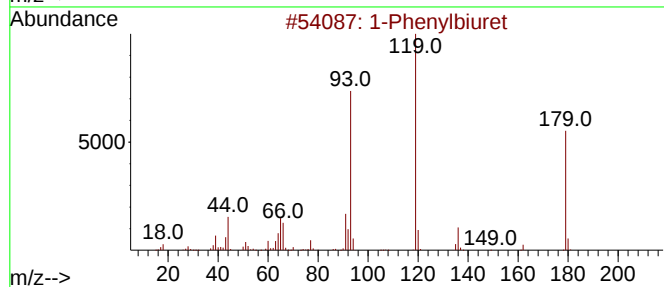
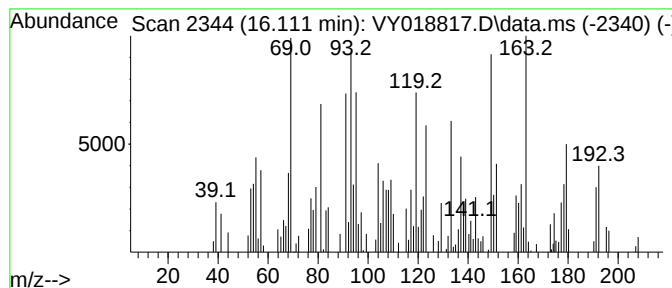
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070924S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown16.110 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.110	5.98 ug/l	47610	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenylbiuret	179	C8H9N3O2	013911-40-5	15
2			2'-Hydroxybutyrophenone oxime	179	C10H13NO2	021667-43-6	15
3			(4-Isobutylphenyl)acetic acid	192	C12H16O2	001553-60-2	15
4			4-Cyclohexylresorcinol	192	C12H16O2	002138-20-7	14
5			[1,3,4]Oxadiazole, 2-amino-5-(4-...	179	C8H6FN3O	1010316-48-2	14



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Instrument :
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ClientSampleId :
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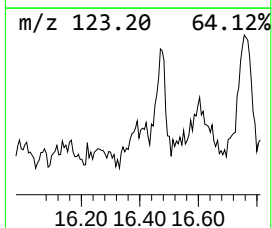
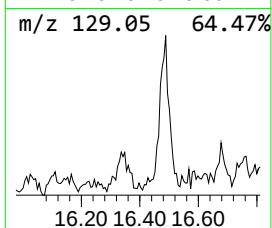
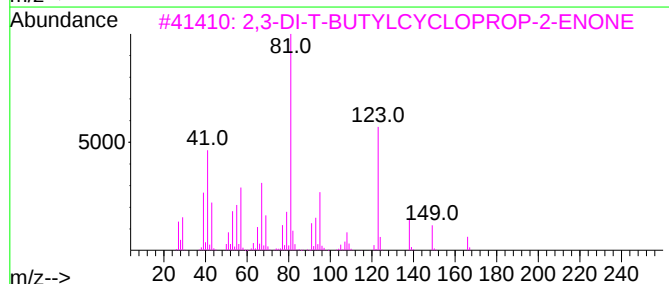
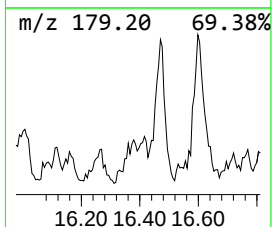
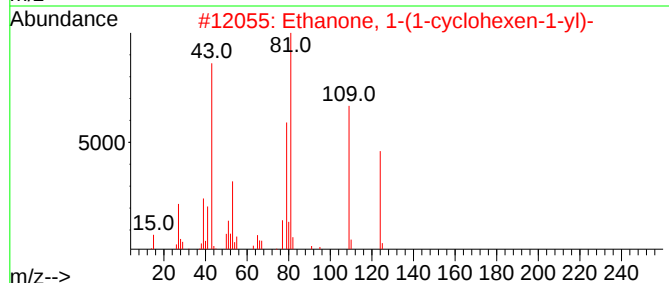
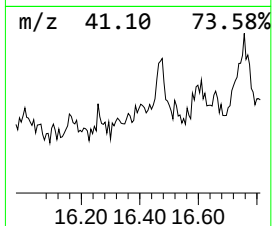
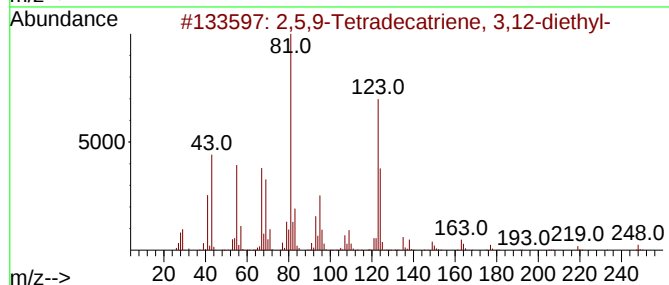
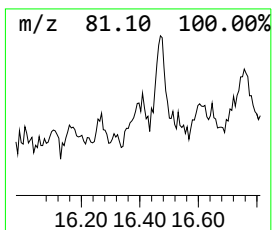
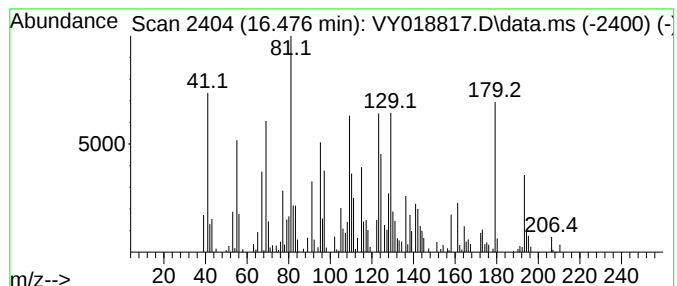
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070924S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown16.476 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.476	14.35 ug/l	114291	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5,9-Tetradecatriene, 3,12-diet...	248	C18H32	074685-87-3	38		
2	Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	000932-66-1	30		
3	2,3-DI-T-BUTYLCYCLOPROP-2-ENONE	166	C11H18O	019985-79-6	30		
4	Cyclopropane, 1,1,2-trimethyl-3...	138	C10H18	054764-57-7	27		
5	2-Cyclopentene-1-acetaldehyde, 2...	166	C10H14O2	075332-42-2	22		



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ClientSampleId :
CHRT-26899RE

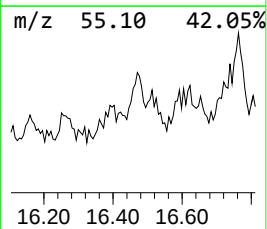
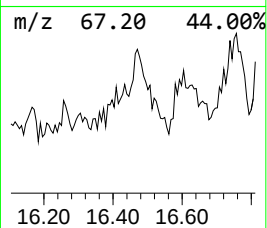
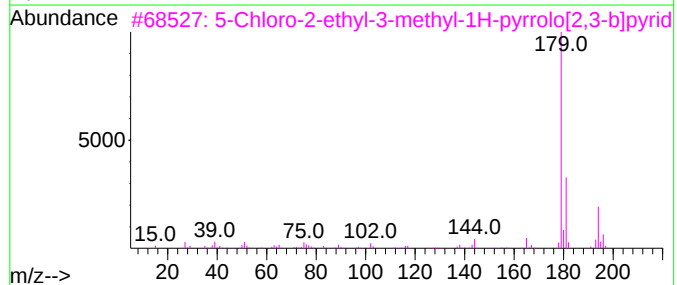
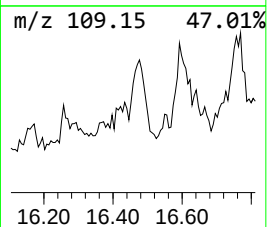
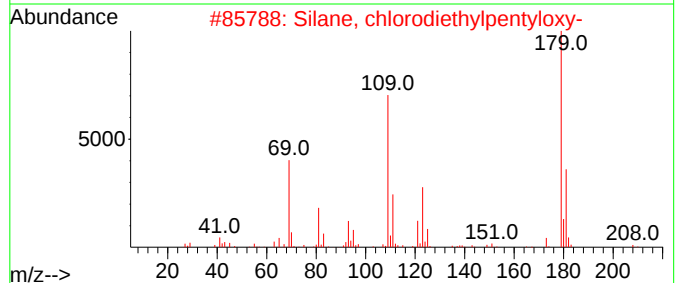
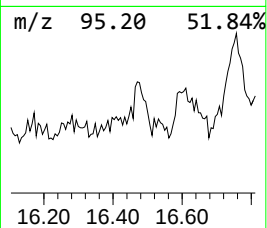
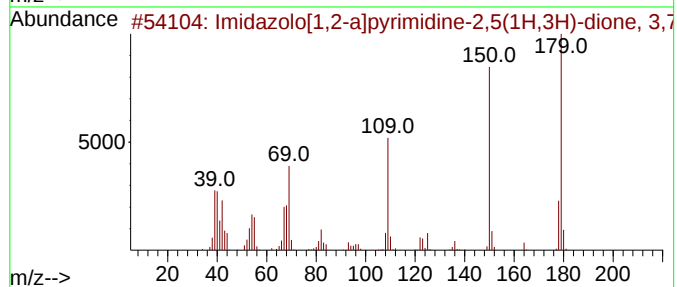
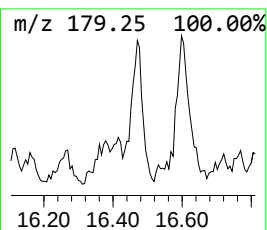
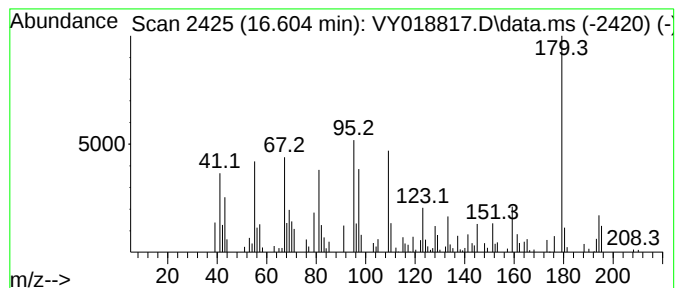
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070924S.M
Quant Title : SW846 8260

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

Peak Number 5 unknown16.604 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.604	16.47 ug/l	131102	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Imidazo[1,2-a]pyrimidine-2,5(1...	179	C8H9N3O2	053854-19-6	35
2			Silane, chlorodiethylpentyloxy-	208	C9H21ClOSi	1000363-04-4	35
3			5-Chloro-2-ethyl-3-methyl-1H-pyr...	194	C10H11ClN2	1000486-81-3	18
4			N,N-Diethyl-3-nitroaniline	194	C10H14N2O2	002216-16-2	18
5			4-Acetyl-7-hydroxybenzo-2,1,3-th...	194	C8H6N2O2S	120893-38-1	18



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071524\
Data File : VY018817.D
Acq On : 15 Jul 2024 17:00
Operator : SY/MD
Sample : P3207-01
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-26899RE

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown14.873	14.873	7.5	ug/l	59332	4	13.422	398113	50.0
unknown15.269	15.269	6.0	ug/l	47609	4	13.422	398113	50.0
unknown16.110	16.110	6.0	ug/l	47610	4	13.422	398113	50.0
unknown16.476	16.476	14.4	ug/l	114291	4	13.422	398113	50.0
unknown16.604	16.604	16.5	ug/l	131102	4	13.422	398113	50.0