

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY100623\
 Data File : VY015871.D
 Acq On : 06 Oct 2023 18:44
 Operator : SY/MD
 Sample : 04778-01
 Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SOIL-1

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\82Y100523S.M
 Title : SW846 8260

Signal : TIC: VY015871.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.954	341	350	367	rBV	15462	44701	1.62%	0.461%
2	4.716	465	475	488	rVB	9397	28318	1.03%	0.292%
3	6.978	835	846	861	rBV2	29245	94823	3.44%	0.977%
4	7.716	954	967	973	rBV2	96727	235013	8.53%	2.423%
5	7.789	973	979	991	rVB	165958	377837	13.72%	3.895%
6	8.137	1021	1036	1046	rBV	105262	241413	8.76%	2.489%
7	8.685	1118	1126	1140	rBV	248485	498583	18.10%	5.140%
8	10.179	1362	1371	1378	rBV	393050	685360	24.88%	7.065%
9	10.575	1428	1436	1442	rBV2	26520	49892	1.81%	0.514%
10	10.941	1489	1496	1503	rBV2	18198	32025	1.16%	0.330%
11	11.490	1578	1586	1596	rBV	351008	597152	21.68%	6.156%
12	12.331	1719	1724	1731	rVB2	39562	66487	2.41%	0.685%
13	12.477	1742	1748	1762	rVB2	316354	531108	19.28%	5.475%
14	13.422	1897	1903	1912	rVB	364946	560257	20.34%	5.775%
15	13.623	1931	1936	1949	rVB	87184	157010	5.70%	1.619%
16	13.886	1970	1979	1988	rBV4	39216	132409	4.81%	1.365%
17	14.264	2035	2041	2044	rBV5	15338	33514	1.22%	0.345%
18	14.385	2050	2061	2074	rVB4	231222	862195	31.30%	8.888%
19	14.727	2104	2117	2129	rVB3	124010	422006	15.32%	4.350%
20	15.233	2192	2200	2209	rBV	1657298	2754697	100.00%	28.397%
21	15.324	2209	2215	2223	rVV2	48447	102071	3.71%	1.052%
22	15.428	2223	2232	2242	rVV2	21411	67863	2.46%	0.700%
23	16.288	2366	2373	2383	rVB	370898	718490	26.08%	7.407%
24	16.483	2398	2405	2414	rVB	194293	407482	14.79%	4.201%

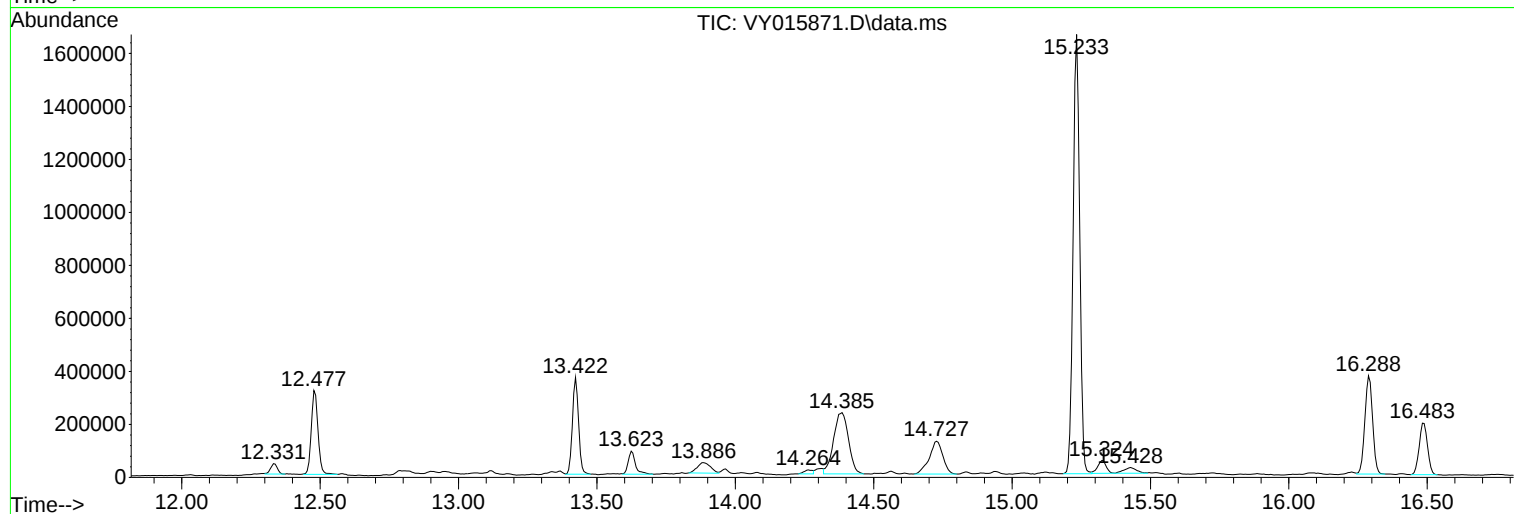
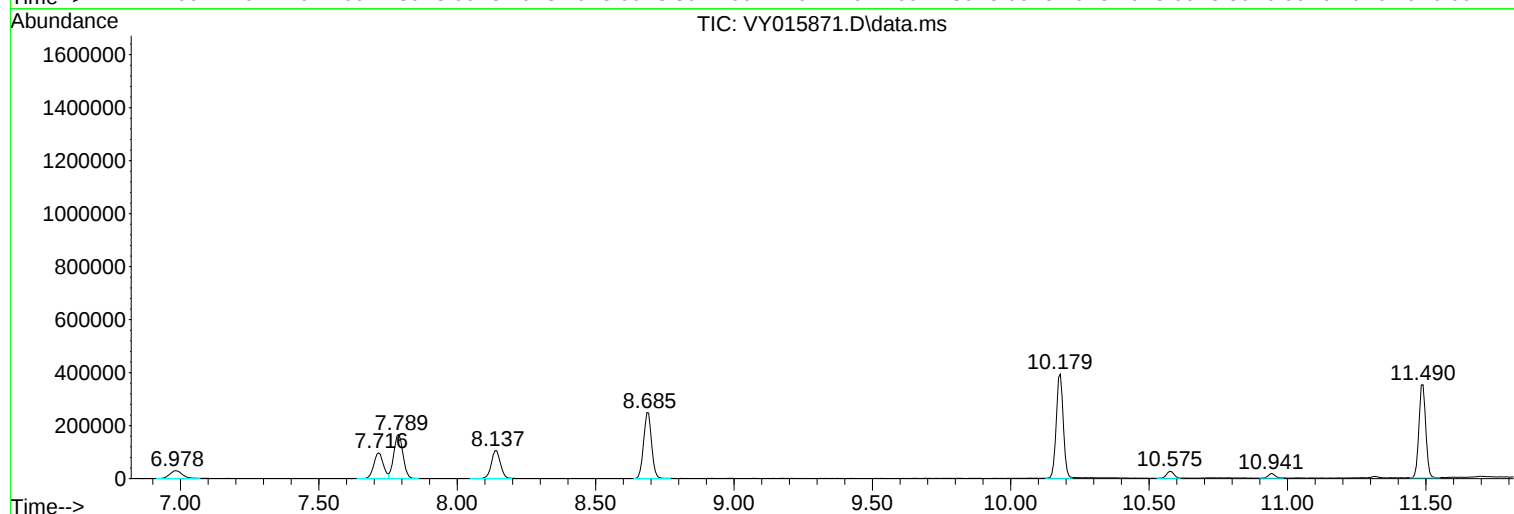
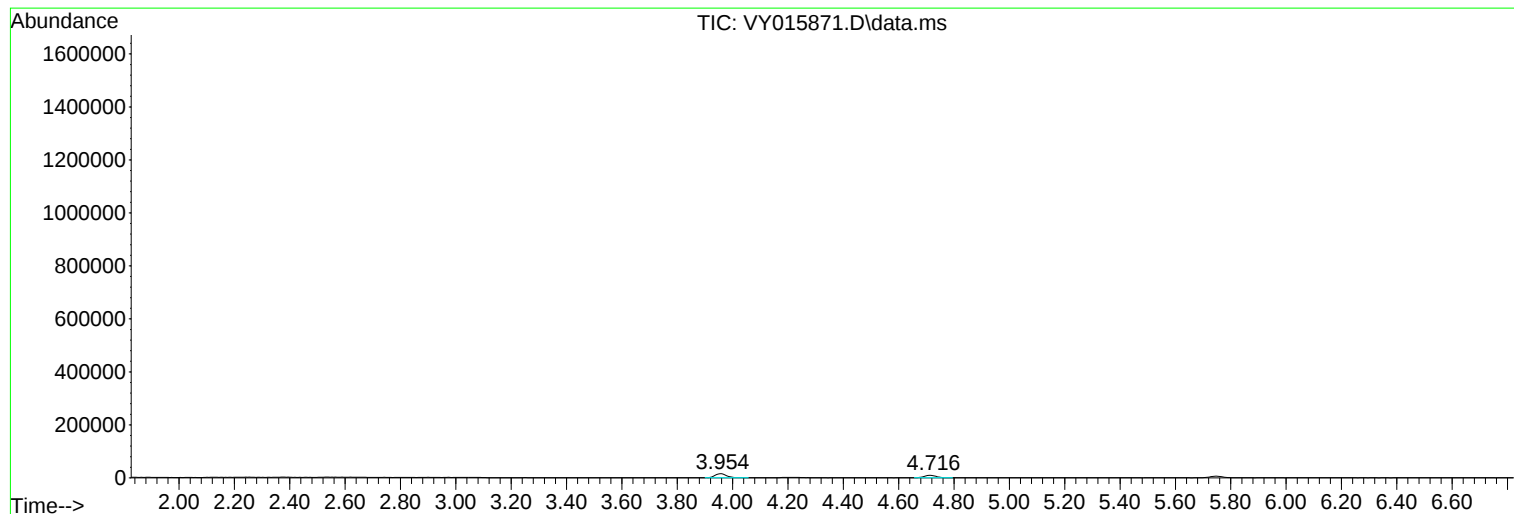
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100523S.M
Quant Title : SW846 8260

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



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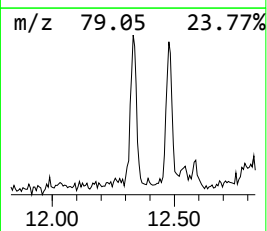
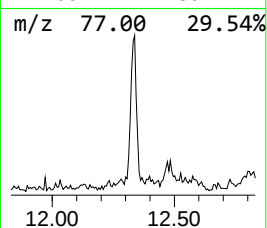
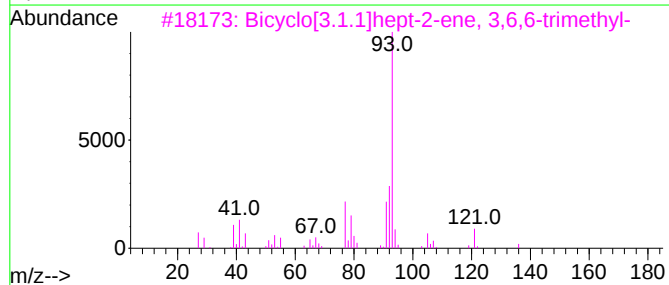
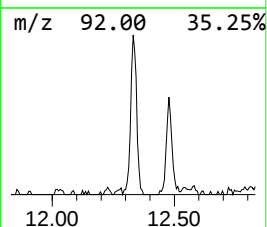
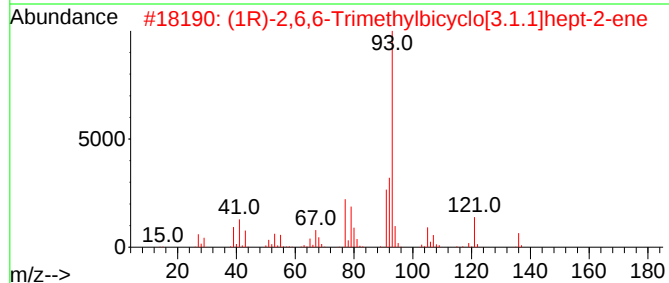
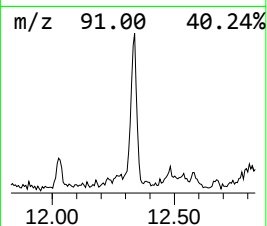
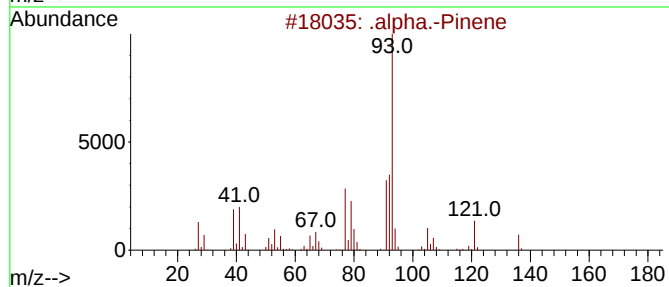
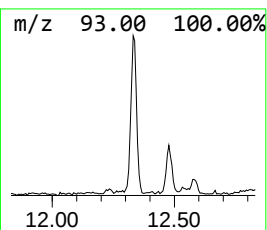
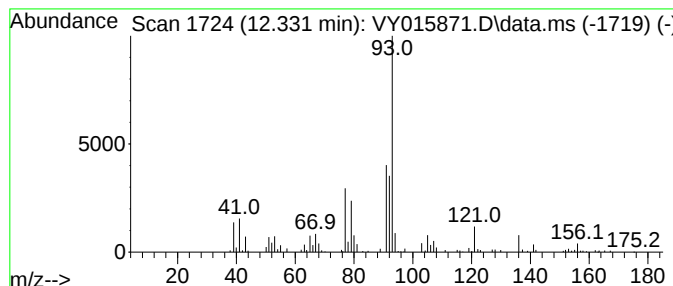
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100523S.M
Quant Title : SW846 8260

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

Peak Number 1 .alpha.-Pinene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.331	5.57 ug/l	66487	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.		.alpha.-Pinene	136	C10H16	000080-56-8	96
2	(1R)-2,6,6-Trimethylbicyclo[3.1....			136	C10H16	007785-70-8	93
3	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...			136	C10H16	004889-83-2	93
4	3-Carene			136	C10H16	013466-78-9	90
5	(1S)-2,6,6-Trimethylbicyclo[3.1....			136	C10H16	007785-26-4	81



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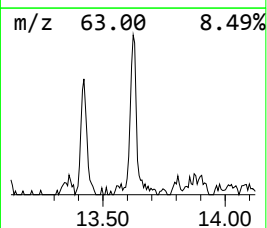
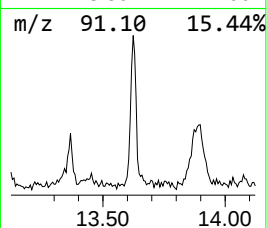
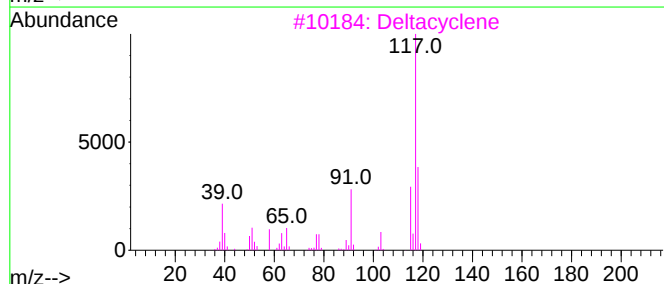
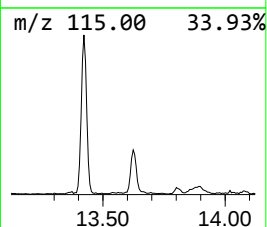
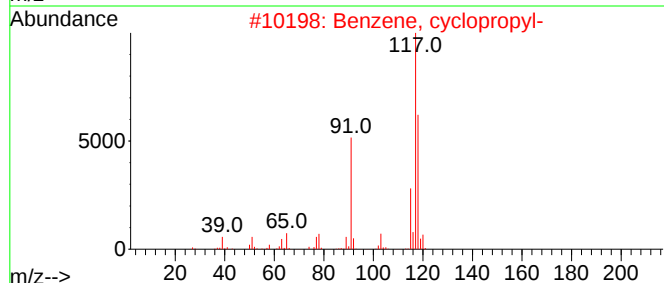
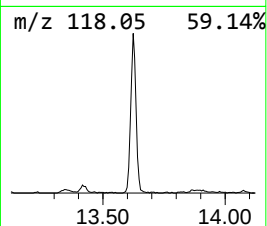
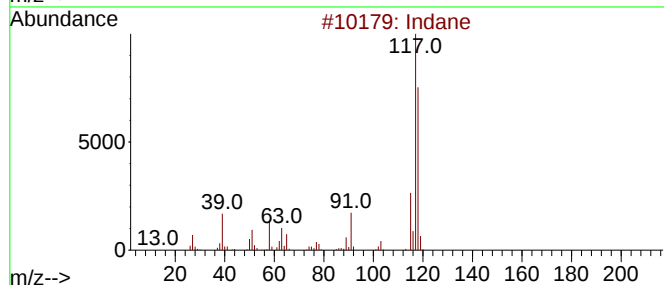
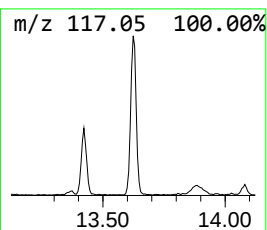
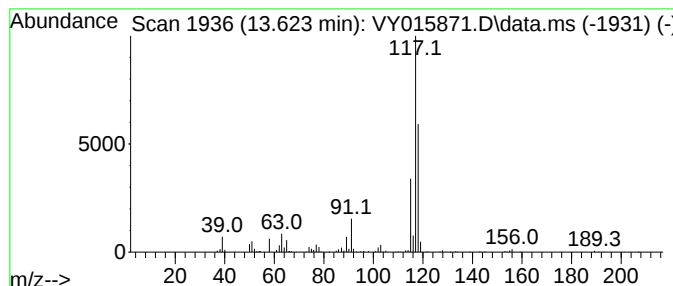
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100523S.M
Quant Title : SW846 8260

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Peak Number 2 Indane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.623	14.01 ug/l	157010	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	91
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	80
3			Deltacyclene	118	C9H10	007785-10-6	72
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	68
5			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	64



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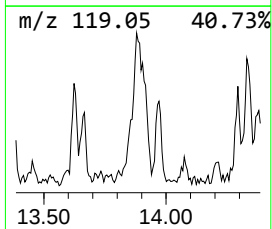
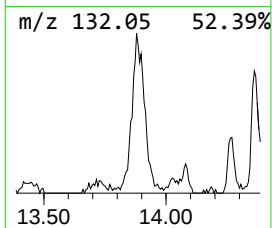
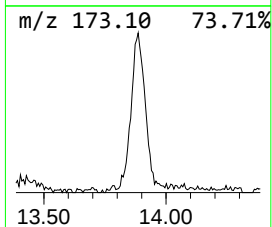
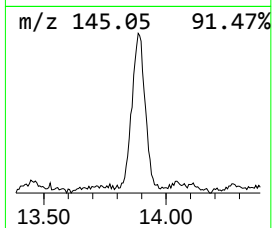
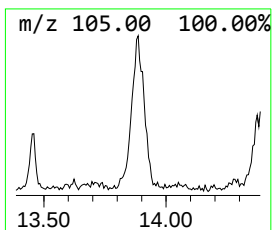
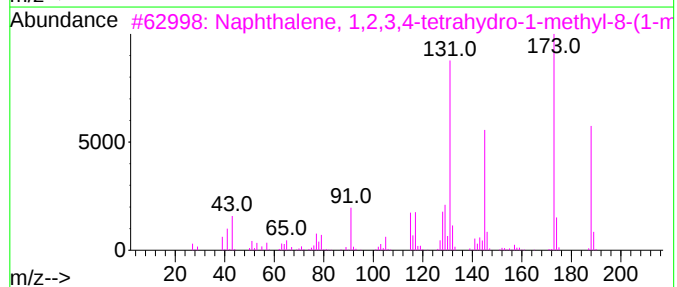
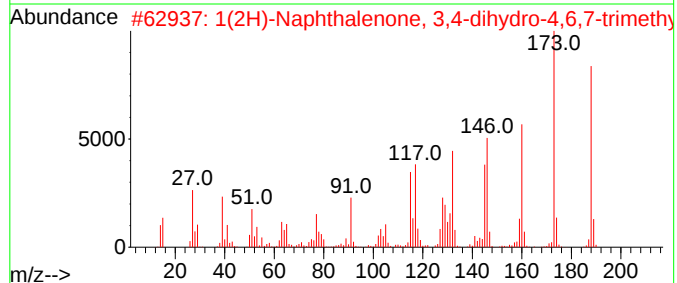
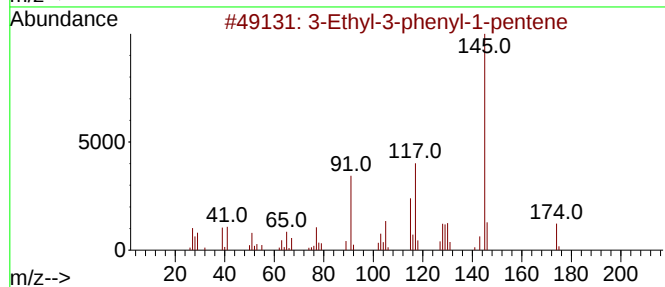
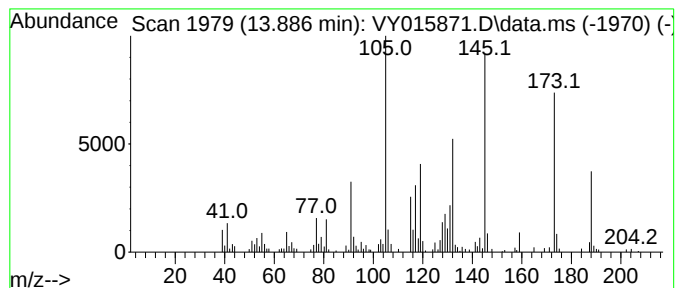
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Quant Title : SW846 8260

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

Peak Number 3 3-Ethyl-3-phenyl-1-pentene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	11.82 ug/l	132409	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Ethyl-3-phenyl-1-pentene	174	C13H18	019781-34-1	70
2			1(2H)-Naphthalenone, 3,4-dihydro...	188	C13H16O	030316-32-6	60
3			Naphthalene, 1,2,3,4-tetrahydro...	188	C14H20	081603-43-2	41
4			1(2H)-Naphthalenone, 3,4-dihydro...	188	C13H16O	030316-31-5	41
5			1-[3-(Trifluoromethyl)phenyl]pen...	228	C12H11F3O	125996-99-8	38



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Instrument :
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ClientSampleId :
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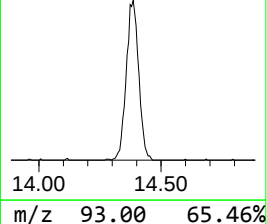
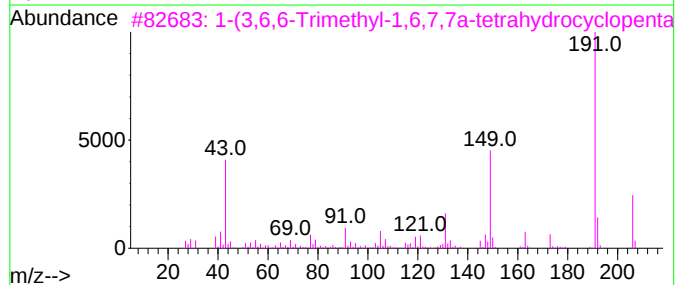
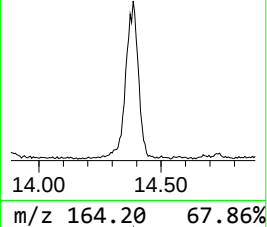
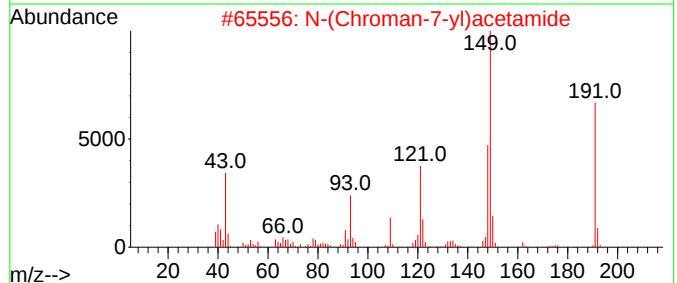
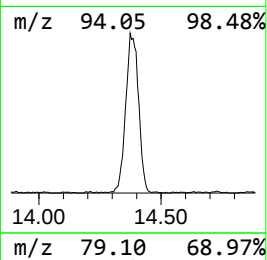
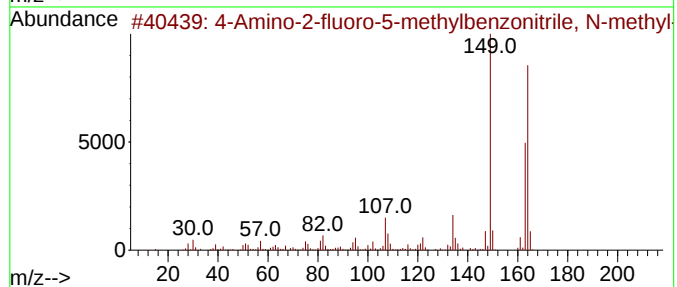
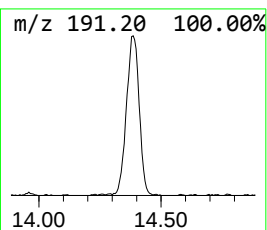
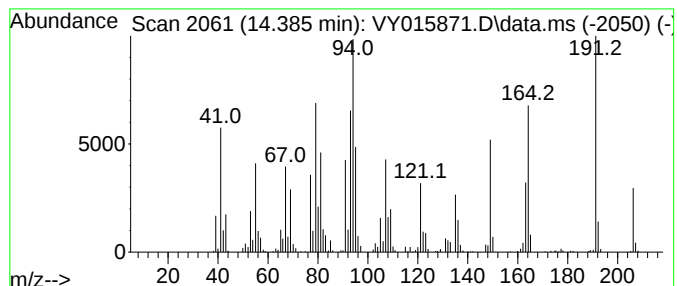
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TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown14.386 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.386	76.95 ug/l	862195	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Amino-2-fluoro-5-methylbenzoni...	164	C9H9FN2	1000511-36-9	42
2			N-(Chroman-7-yl)acetamide	191	C11H13NO2	1000306-69-7	38
3			1-(3,6,6-Trimethyl-1,6,7,7a-tetr...	206	C13H18O2	1000194-97-2	38
4			4(1H)-Azulenone, octahydro-1-met...	164	C11H16O	111615-51-1	35
5			Oxirane, [[4-(1,1-dimethylethyl)...]	206	C13H18O2	003101-60-8	30



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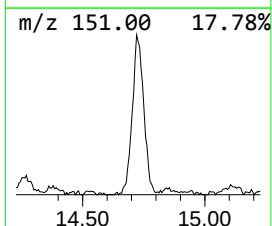
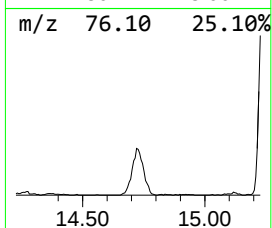
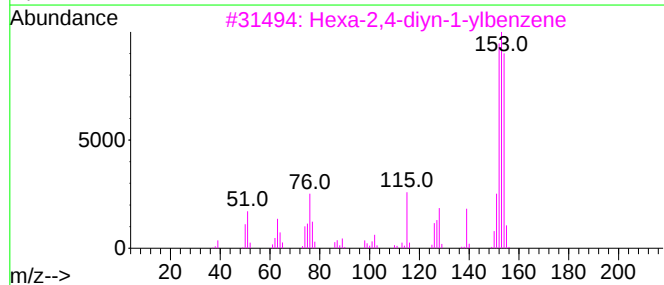
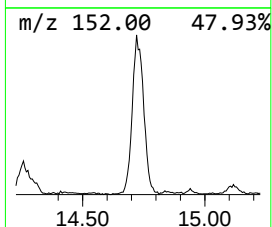
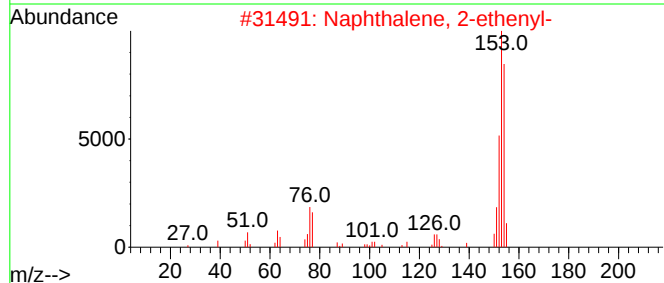
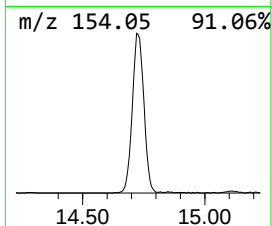
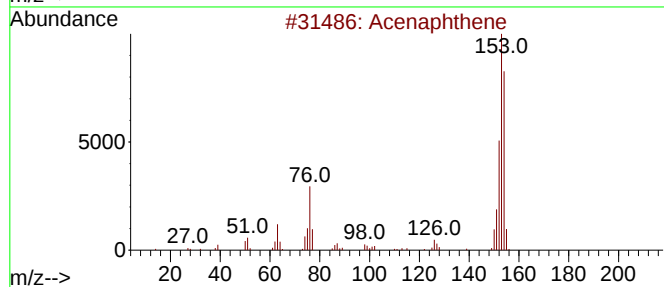
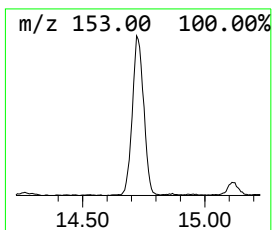
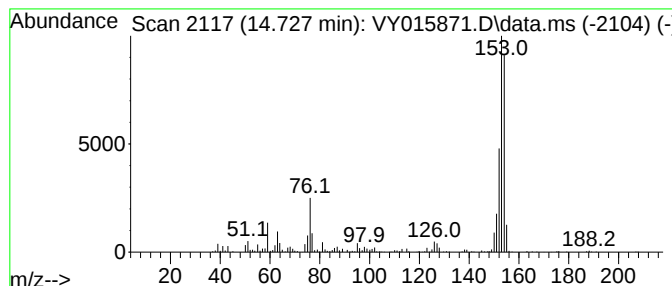
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexa-2,4-diyn-1-ylbenzene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.727	37.66 ug/l	422006	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	96
2			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	64
3			Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	59
4			1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	53
5			2,4,6-Trihydroxybenzaldehyde	154	C7H6O4	000487-70-7	47



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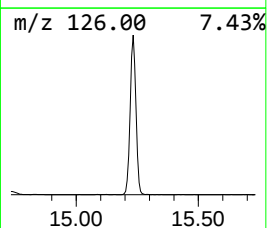
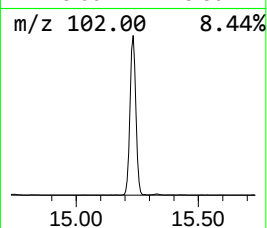
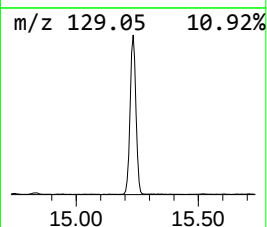
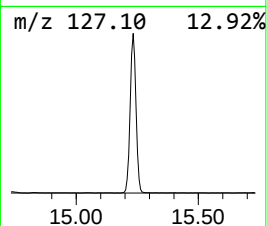
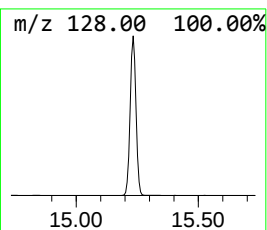
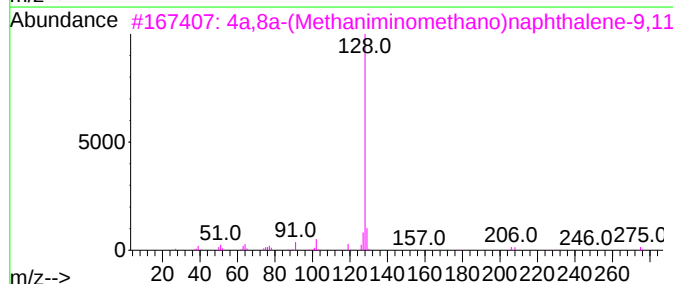
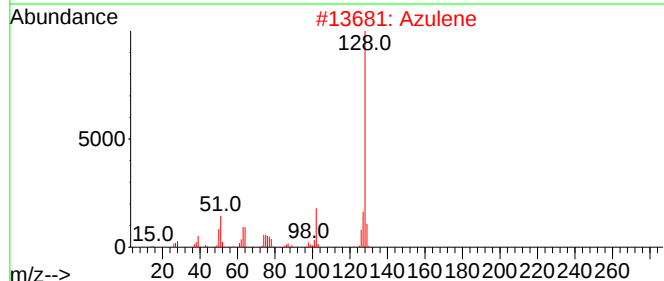
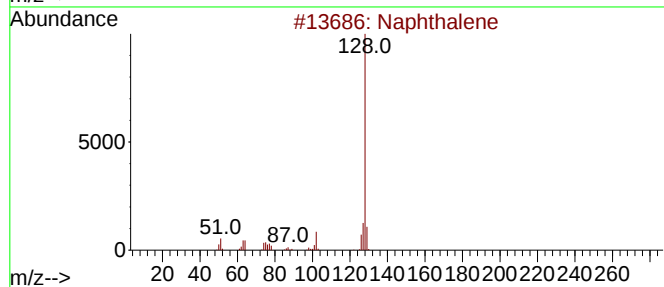
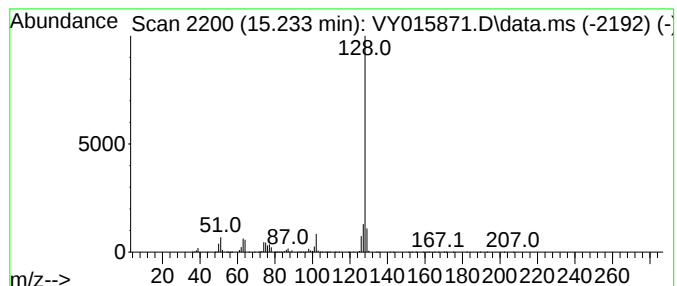
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Quant Title : SW846 8260

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

Peak Number 6 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.233	245.84 ug/l	2754700	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	91
3			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	78
4			[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	50
5			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY100623\
Data File : VY015871.D
Acq On : 06 Oct 2023 18:44
Operator : SY/MD
Sample : 04778-01
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SOIL-1

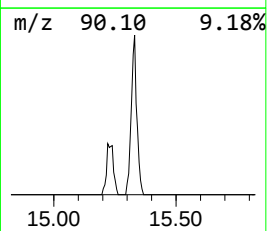
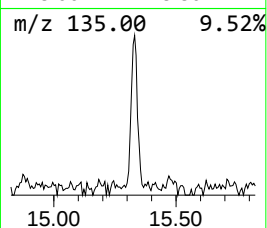
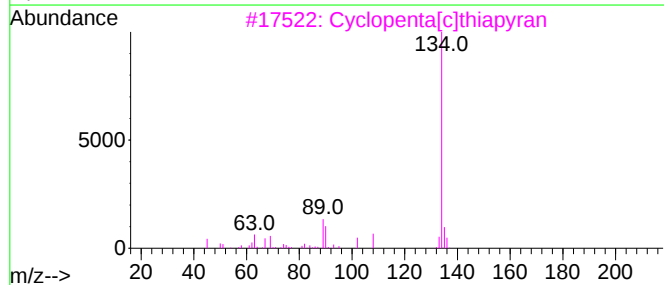
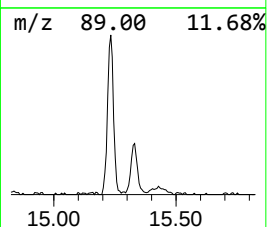
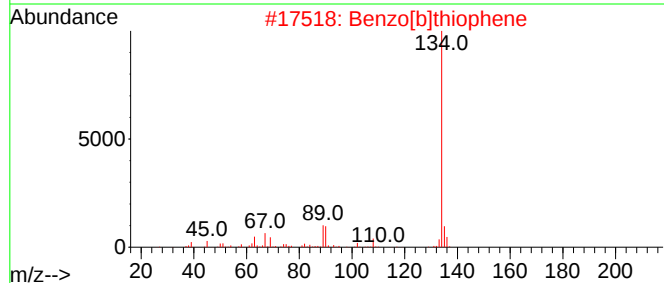
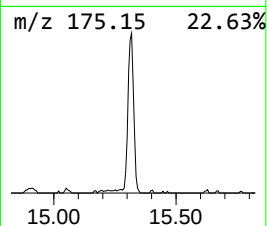
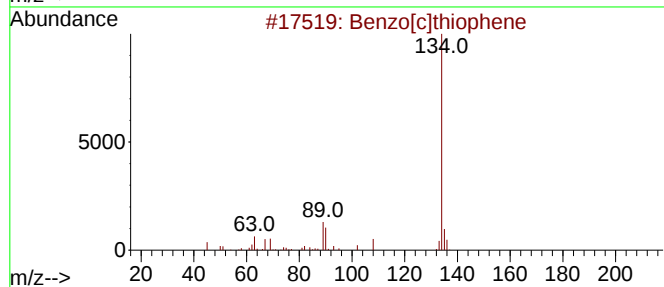
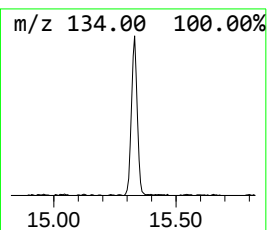
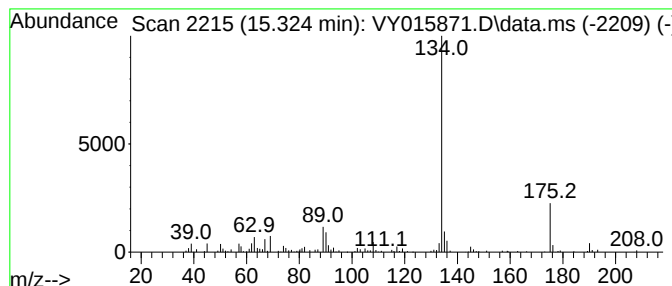
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Quant Title : SW846 8260

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

Peak Number 7 Benzo[c]thiophene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.324	9.11 ug/l	102071	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]thiophene	134	C8H6S	000270-82-6	94
2			Benzo[b]thiophene	134	C8H6S	000095-15-8	93
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	90
4			Thiazole, 2-methyl-4-phenyl-	175	C10H9NS	001826-16-0	87
5			3-Deazaadenine	134	C6H6N4	006811-77-4	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY100623\
Data File : VY015871.D
Acq On : 06 Oct 2023 18:44
Operator : SY/MD
Sample : 04778-01
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SOIL-1

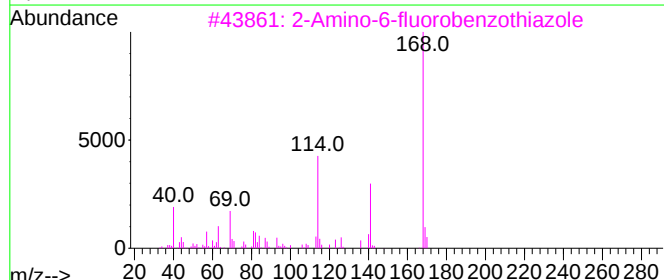
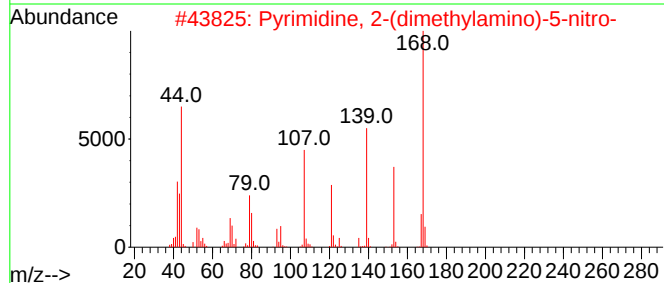
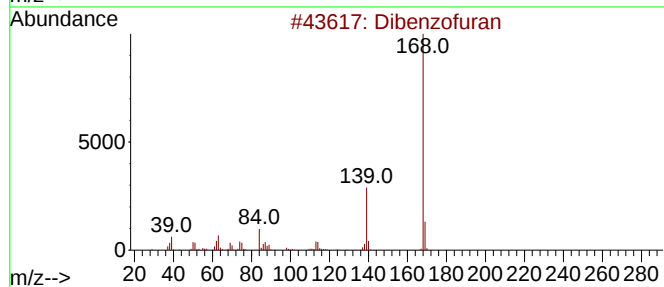
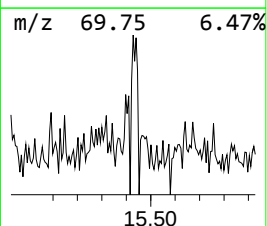
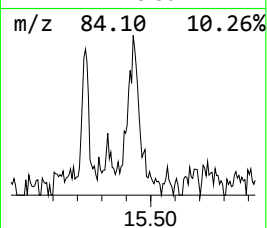
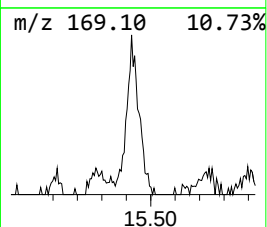
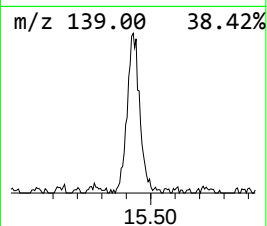
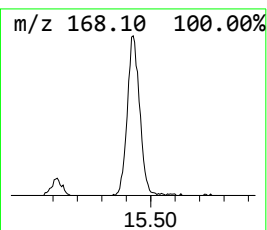
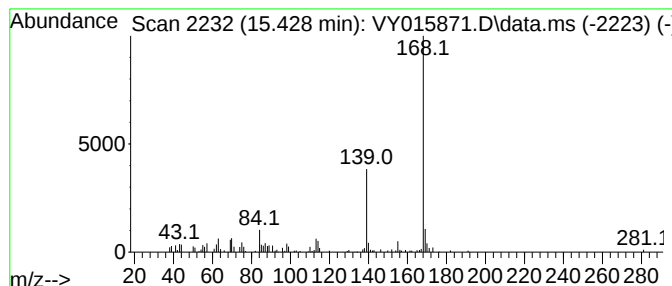
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Quant Title : SW846 8260

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

Peak Number 8 Dibenzofuran Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.428	6.06 ug/l	67863	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzofuran	168	C12H8O	000132-64-9	90
2			Pyrimidine, 2-(dimethylamino)-5-...	168	C6H8N4O2	014233-44-4	64
3			2-Amino-6-fluorobenzothiazole	168	C7H5FN2S	000348-40-3	49
4			Naphtho[2,1-d]imidazole	168	C11H8N2	000233-53-4	49
5			Quinoline-4-carbonitrile, 2-methyl-	168	C11H8N2	1000317-19-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY100623\
Data File : VY015871.D
Acq On : 06 Oct 2023 18:44
Operator : SY/MD
Sample : 04778-01
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SOIL-1

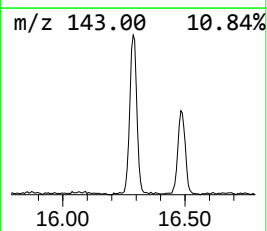
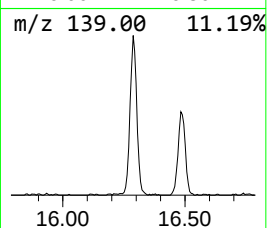
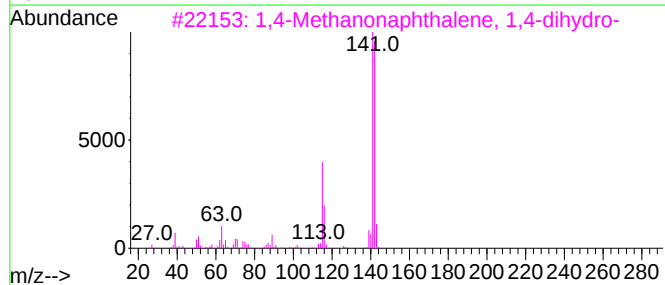
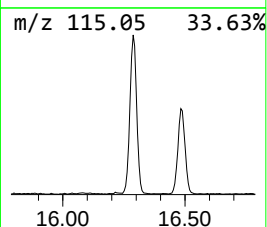
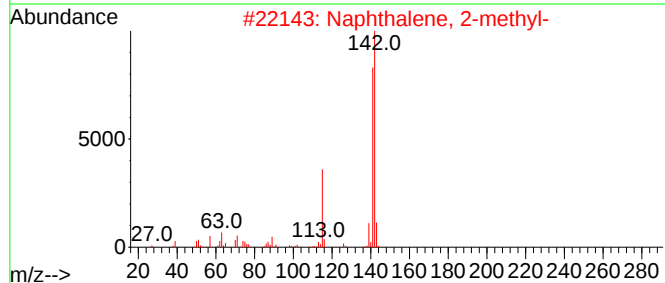
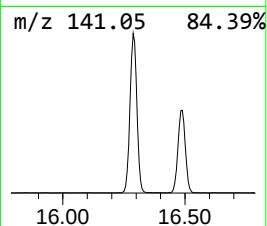
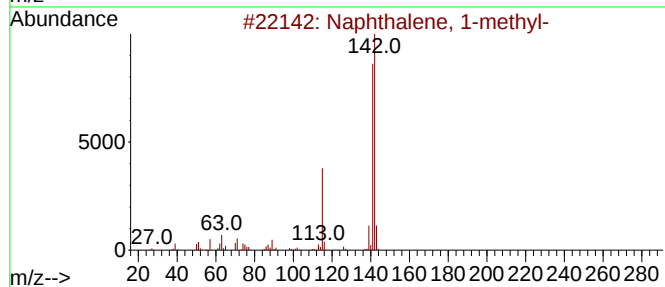
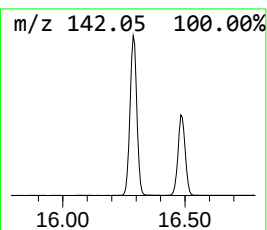
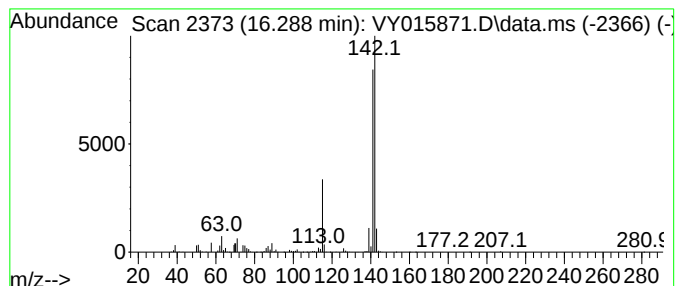
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100523S.M
Quant Title : SW846 8260

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

Peak Number 9 1,4-Methanonaphthalene, 1,4... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.288	64.12 ug/l	718490	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			2-Naphthaleneethanol	172	C12H12O	001485-07-0	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY100623\
Data File : VY015871.D
Acq On : 06 Oct 2023 18:44
Operator : SY/MD
Sample : 04778-01
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SOIL-1

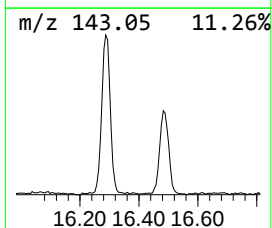
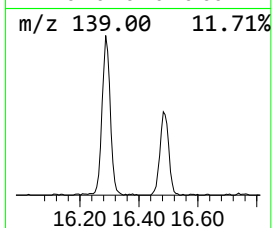
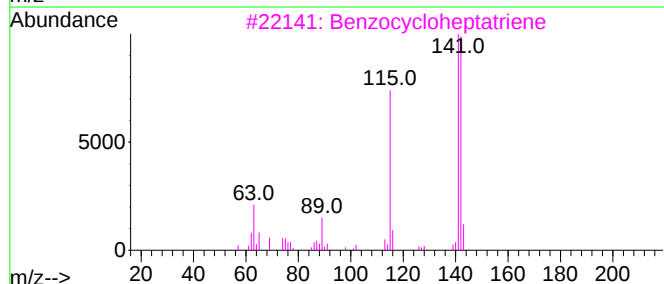
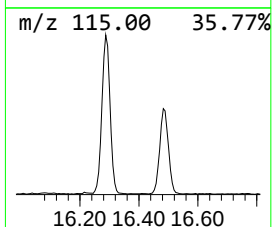
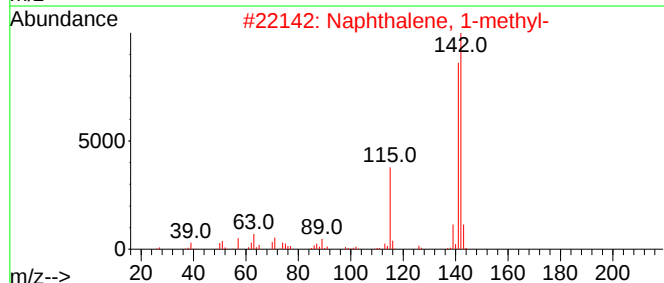
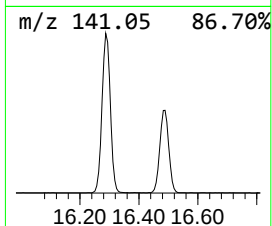
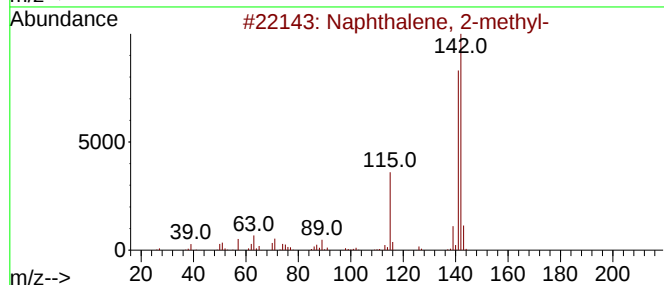
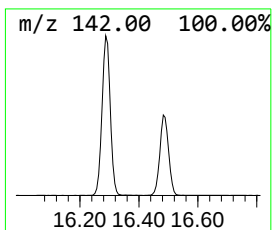
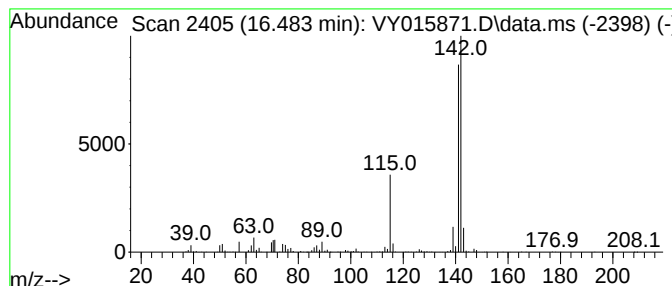
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100523S.M
Quant Title : SW846 8260

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

Peak Number 10 Benzocycloheptatriene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.483	36.37 ug/l	407482	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	90
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY100623\
Data File : VY015871.D
Acq On : 06 Oct 2023 18:44
Operator : SY/MD
Sample : 04778-01
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SOIL-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100523S.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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Indane	13.623	14.0	ug/l	157010	4	13.422	560257	50.0
3-Ethyl-3-pheny...	13.886	11.8	ug/l	132409	4	13.422	560257	50.0
unknown14.386	14.386	77.0	ug/l	862195	4	13.422	560257	50.0
Hexa-2,4-diyn-1...	14.727	37.7	ug/l	422006	4	13.422	560257	50.0
Azulene	15.233	245.8	ug/l	2754700	4	13.422	560257	50.0
Benzo[c]thiophene	15.324	9.1	ug/l	102071	4	13.422	560257	50.0
Dibenzofuran	15.428	6.1	ug/l	67863	4	13.422	560257	50.0
1,4-Methanonaph...	16.288	64.1	ug/l	718490	4	13.422	560257	50.0
Benzocyclohepta...	16.483	36.4	ug/l	407482	4	13.422	560257	50.0