

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY100623\
 Data File : VY015873.D
 Acq On : 06 Oct 2023 19:32
 Operator : SY/MD
 Sample : 04778-07
 Misc : 4.55g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SOIL-3

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: VY015873.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.972	341	353	368	rBV	21370	83603	1.01%	0.366%
2	6.996	837	849	868	rBV3	41583	146296	1.76%	0.641%
3	7.716	958	967	973	rBV	247351	599261	7.21%	2.624%
4	7.789	973	979	993	rVB	429737	940830	11.32%	4.120%
5	8.142	1024	1037	1049	rBV	275197	608805	7.33%	2.666%
6	8.691	1114	1127	1146	rBV	642586	1286522	15.49%	5.633%
7	10.179	1362	1371	1380	rBV	1021205	1742198	20.97%	7.629%
8	11.489	1578	1586	1598	rBV	958446	1556390	18.73%	6.815%
9	12.331	1718	1724	1730	rBV	60602	98638	1.19%	0.432%
10	12.477	1741	1748	1756	rBV	786475	1273042	15.32%	5.574%
11	13.422	1897	1903	1918	rVB	987743	1536591	18.50%	6.728%
12	13.623	1929	1936	1949	rVB	276341	438526	5.28%	1.920%
13	14.684	2102	2110	2113	rBV2	43928	85668	1.03%	0.375%
14	14.733	2113	2118	2128	rVB2	58310	112354	1.35%	0.492%
15	15.233	2192	2200	2208	rVV	5065945	8308046	100.00%	36.379%
16	15.330	2208	2216	2223	rVB	140421	273884	3.30%	1.199%
17	16.287	2366	2373	2386	rVB	1204054	2368196	28.50%	10.370%
18	16.482	2397	2405	2419	rVB	660972	1378405	16.59%	6.036%

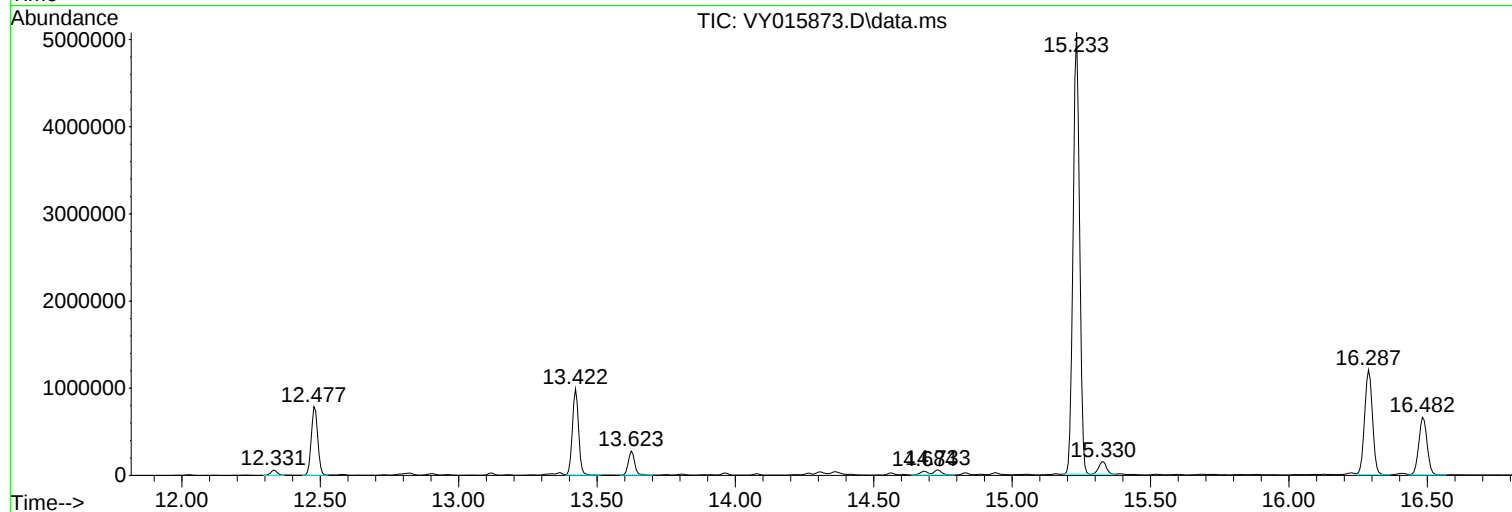
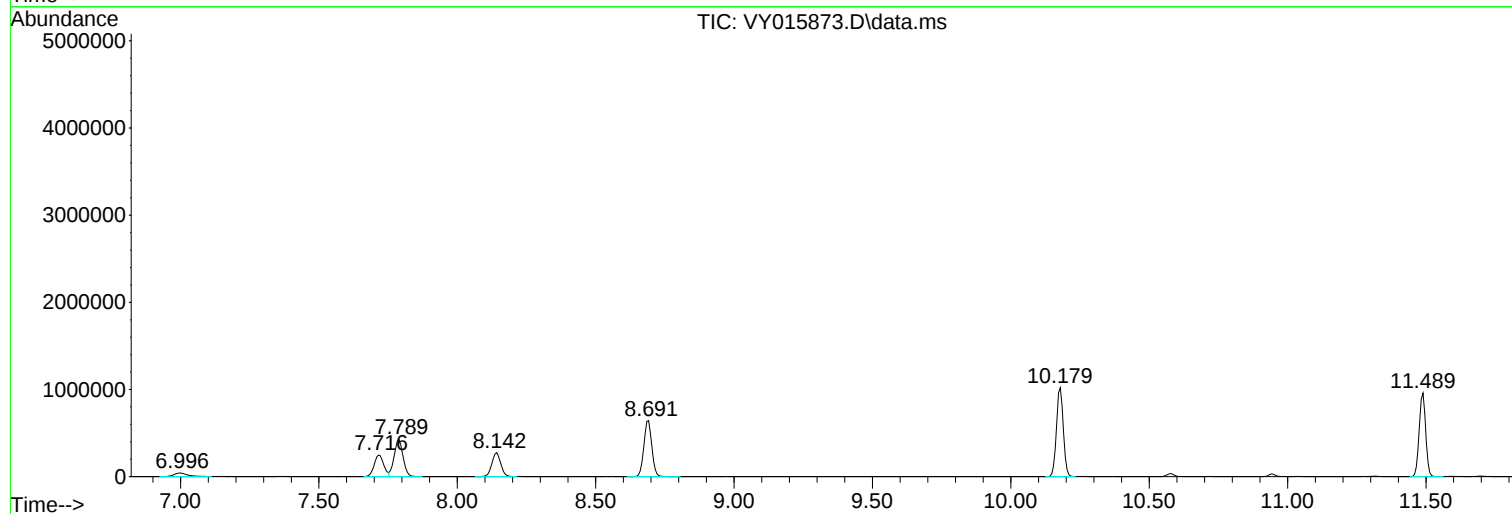
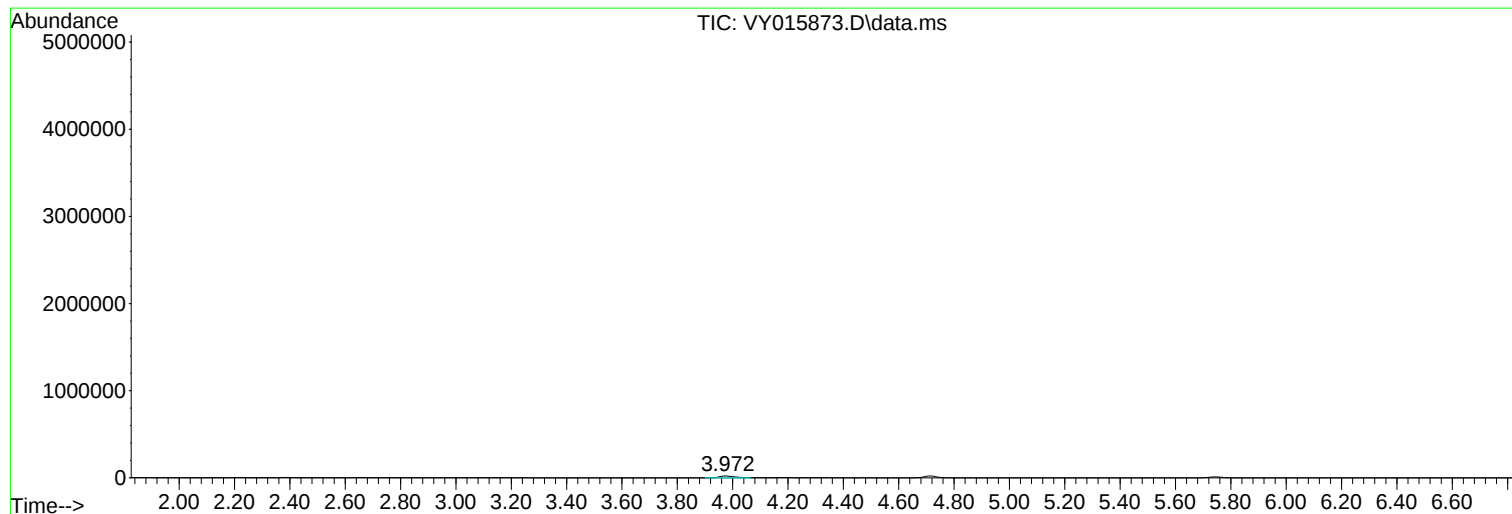
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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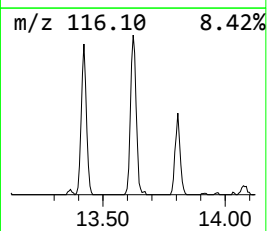
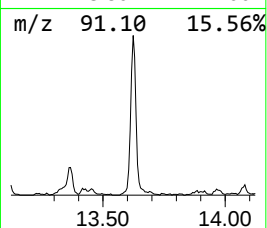
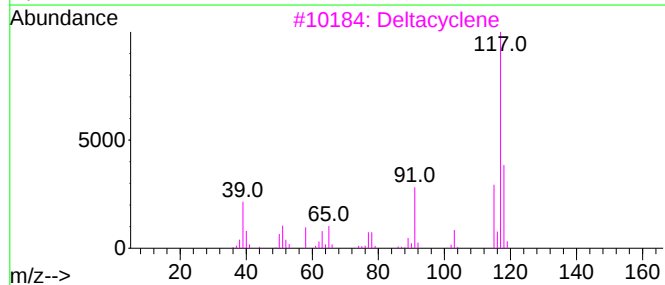
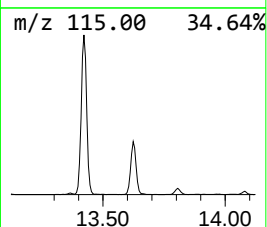
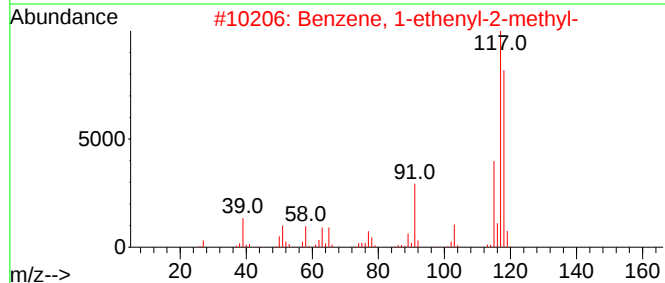
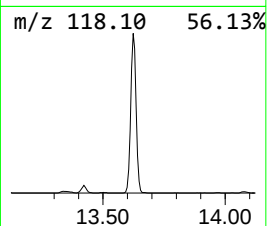
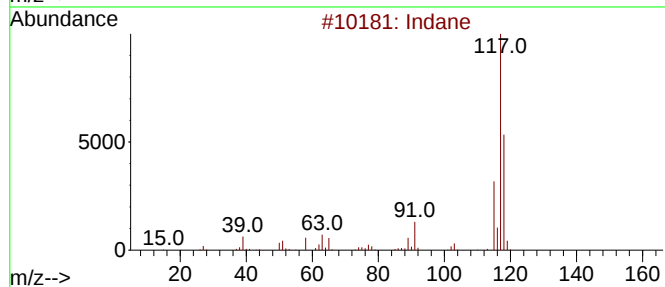
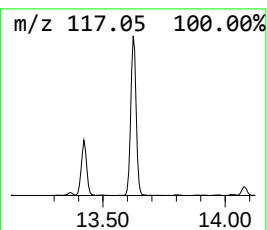
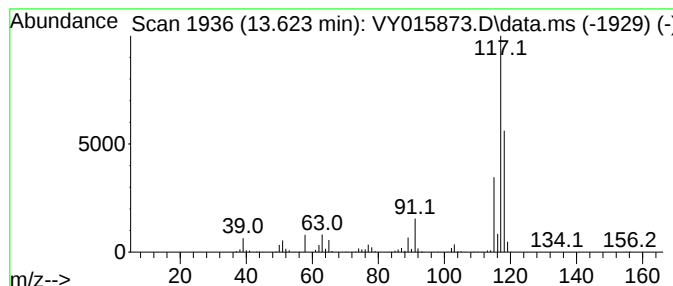
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100523S.M
Quant Title : SW846 8260

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

Peak Number 1 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.623	14.27 ug/l	438526	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	95
2			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	78
3			Deltacyclene	118	C9H10	007785-10-6	72
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	53



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MSVOA_Y
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SOIL-3

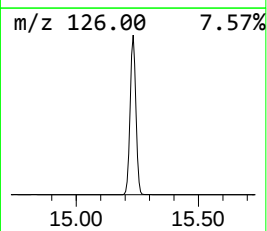
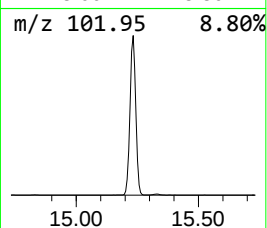
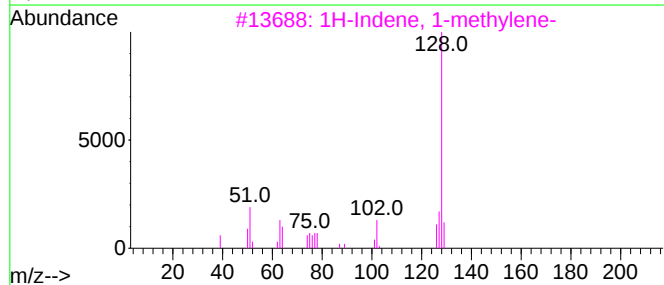
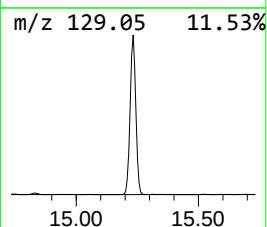
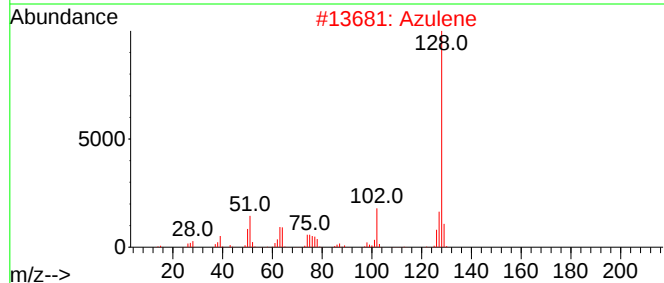
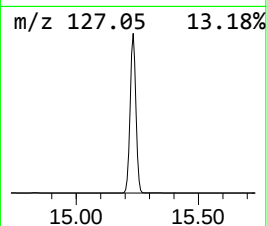
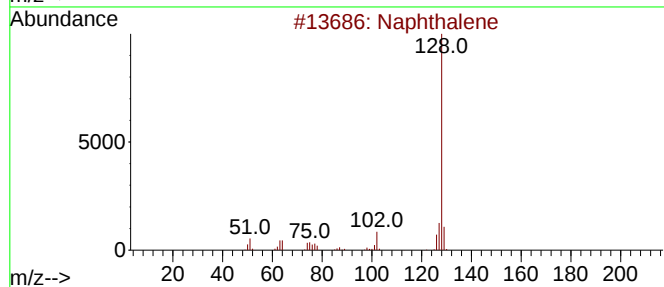
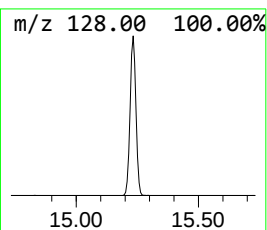
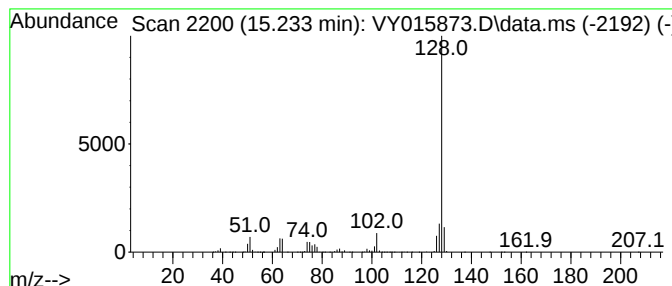
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100523S.M
Quant Title : SW846 8260

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

Peak Number 2 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.233	270.34 ug/l	8308050	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			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	91
4			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	64
5			Tetracyanoethylene	128	C6N4	000670-54-2	45



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Instrument :
MSVOA_Y
ClientSampleId :
SOIL-3

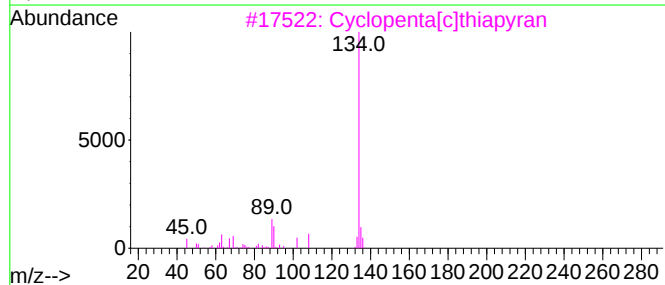
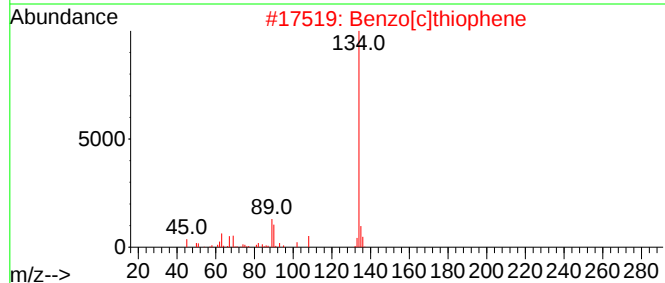
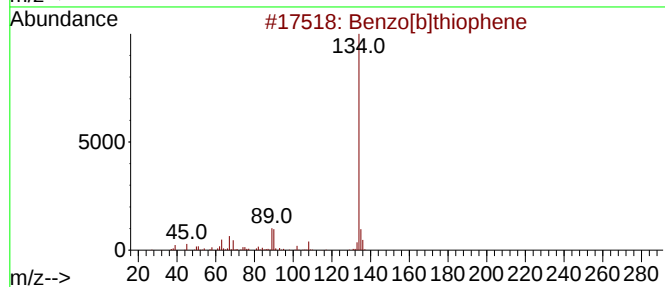
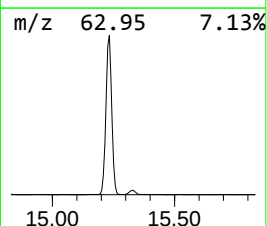
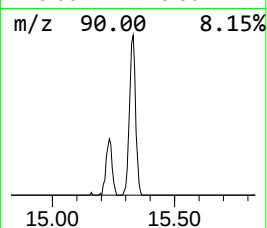
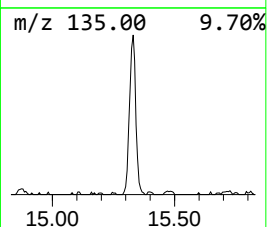
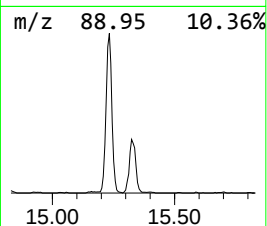
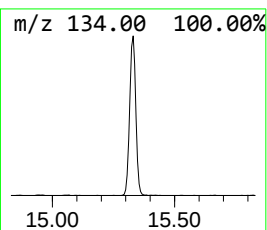
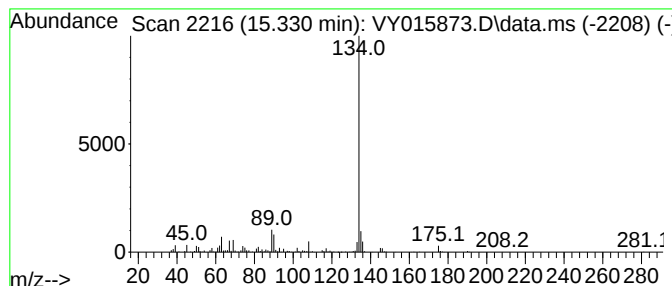
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzo[b]thiophene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.330	8.91 ug/l	273884	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]thiophene	134	C8H6S	000095-15-8	95
2			Benzo[c]thiophene	134	C8H6S	000270-82-6	95
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	94
4			5H-Pyrrolo(3,2-d)pyrimidin-4-amine	134	C6H6N4	002227-98-7	45
5			Thiazolidin-4-one, 5-benzylideno...	287	C13H9N3OS2	351062-07-2	45



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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SOIL-3

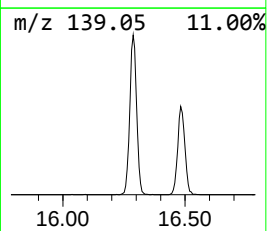
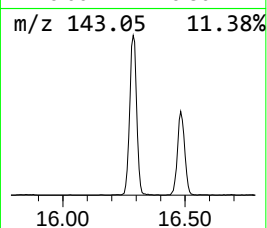
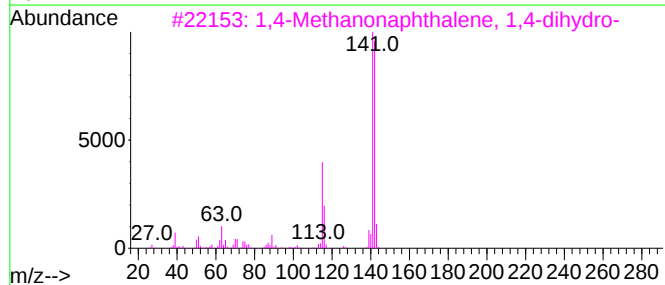
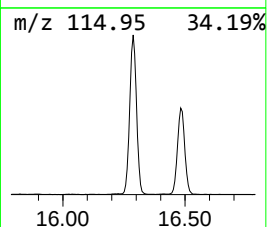
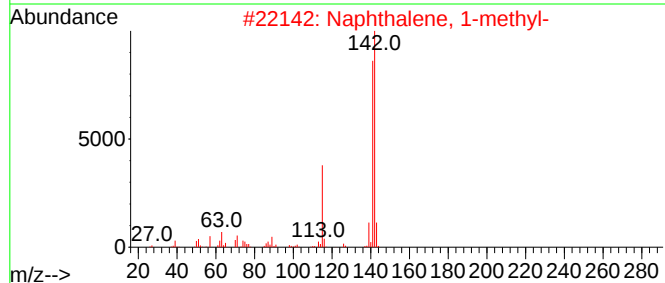
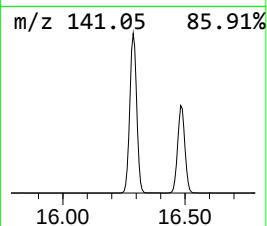
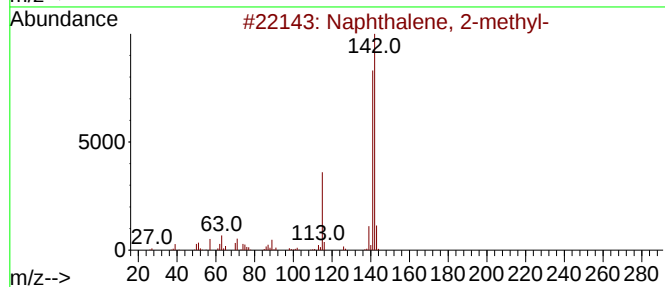
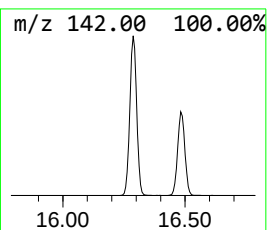
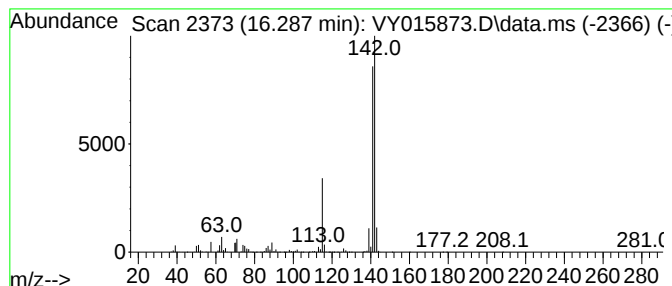
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1,4-Methanonaphthalene, 1,4... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.287	77.06 ug/l	2368200	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			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	49



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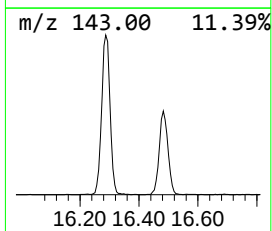
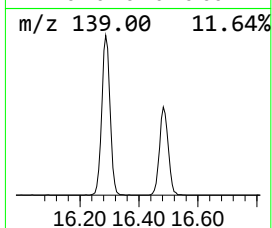
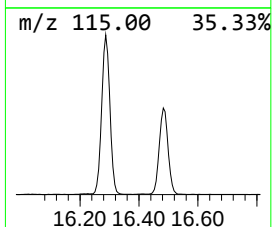
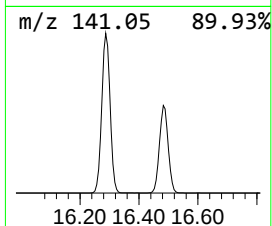
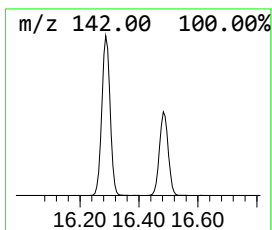
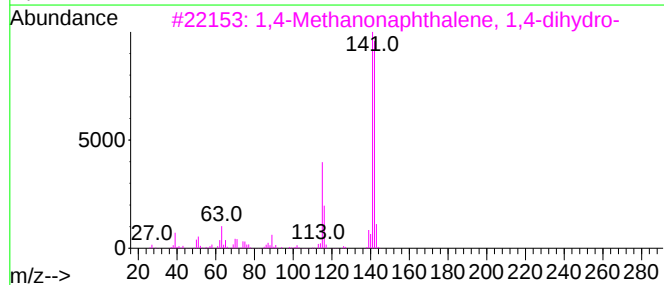
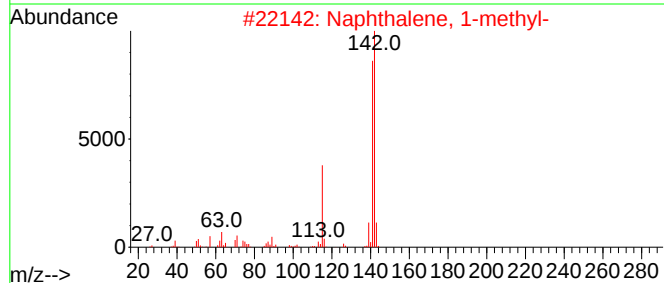
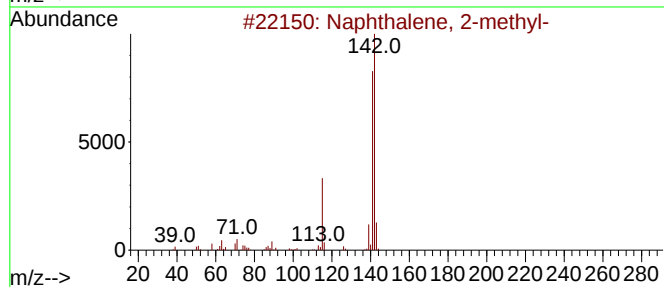
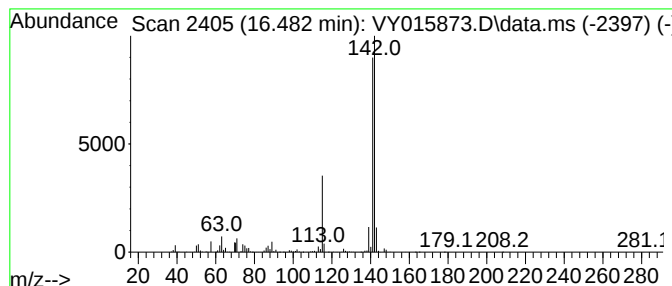
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzocycloheptatriene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.482	44.85 ug/l	1378410	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			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	64



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Indane	13.623	14.3	ug/l	438526	4	13.422	1536590	50.0
Azulene	15.233	270.3	ug/l	8308050	4	13.422	1536590	50.0
Benzo[b]thiophene	15.330	8.9	ug/l	273884	4	13.422	1536590	50.0
1,4-Methanonaph...	16.287	77.1	ug/l	2368200	4	13.422	1536590	50.0
Benzocyclohepta...	16.482	44.9	ug/l	1378410	4	13.422	1536590	50.0