

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071124\
 Data File : VY018782.D
 Acq On : 11 Jul 2024 16:49
 Operator : SY/MD
 Sample : P3223-02
 Misc : 3.00g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 PILE-CAP

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: VY018782.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.180	376	387	397	rVB	7284	19444	1.60%	0.814%
2	7.710	957	966	971	rBV3	18056	42926	3.52%	1.797%
3	7.777	971	977	990	rVB2	33284	76901	6.31%	3.220%
4	8.130	1025	1035	1043	rBV2	15115	35376	2.90%	1.481%
5	8.679	1116	1125	1133	rBV	48238	101262	8.31%	4.240%
6	10.173	1364	1370	1377	rBV	70646	125569	10.31%	5.258%
7	11.490	1580	1586	1592	rBV	59093	100223	8.23%	4.197%
8	12.032	1668	1675	1678	rBV5	30189	74601	6.12%	3.124%
9	12.337	1721	1725	1729	rBV5	12399	22982	1.89%	0.962%
10	12.483	1744	1749	1753	rBV2	50009	88631	7.27%	3.711%
11	13.623	1933	1936	1942	rVB2	39427	58662	4.81%	2.456%
12	13.751	1951	1957	1964	rBV2	31427	91364	7.50%	3.826%
13	13.959	1989	1991	1996	rVB2	23641	33584	2.76%	1.406%
14	14.245	2026	2038	2056	rVB2	340586	1218397	100.00%	51.017%
15	14.916	2143	2148	2160	rVB3	60796	188780	15.49%	7.905%
16	15.227	2196	2199	2208	rVB4	47118	109510	8.99%	4.585%

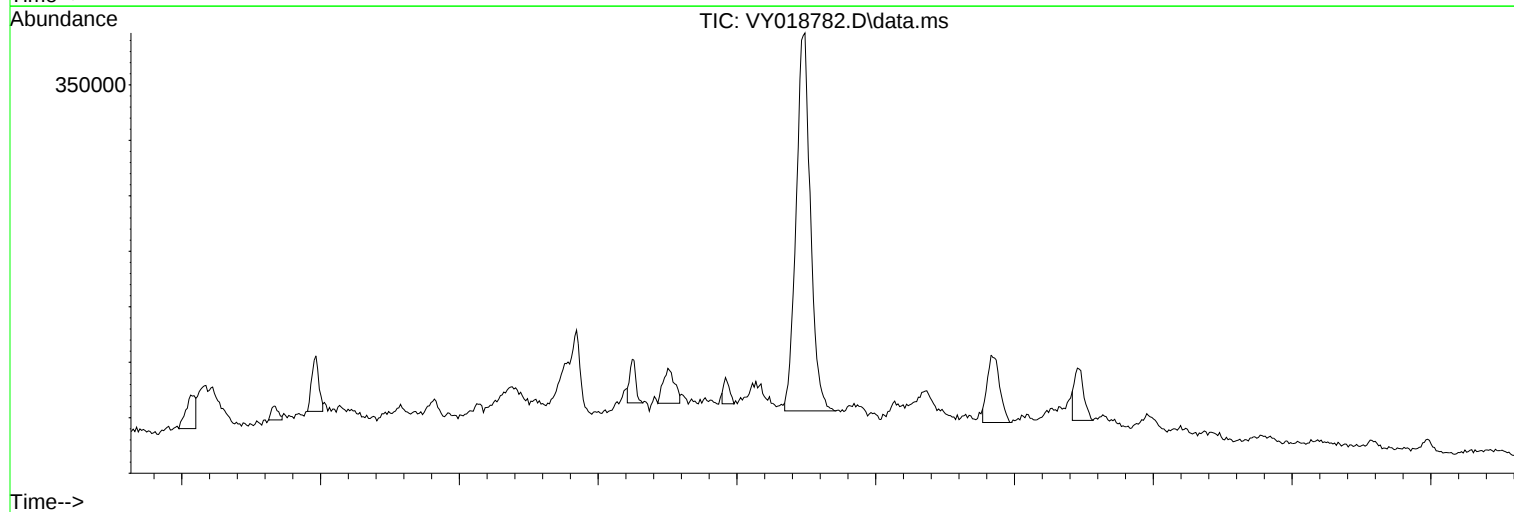
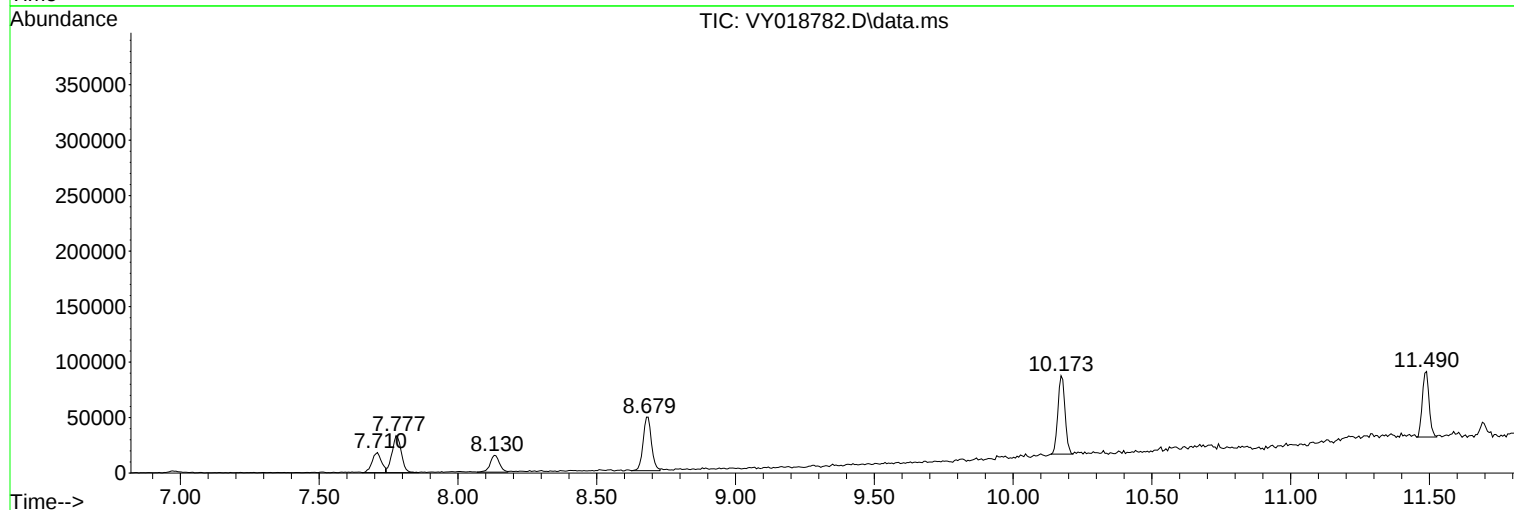
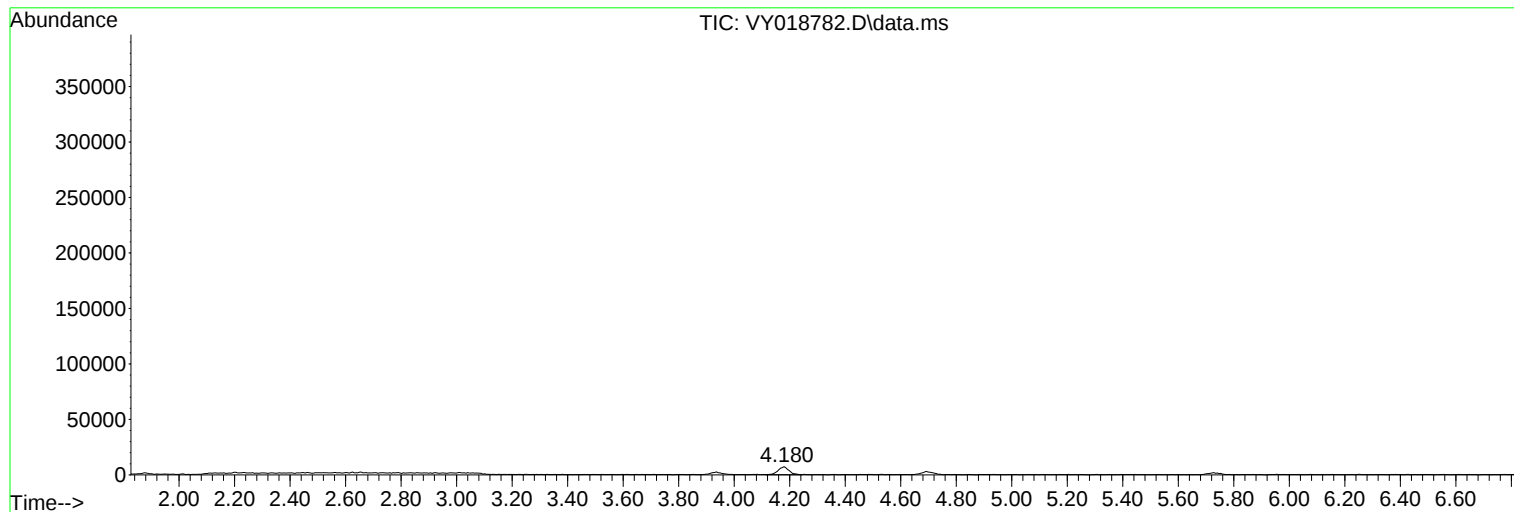
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PILE-CAP

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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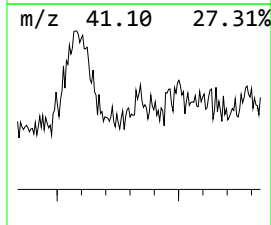
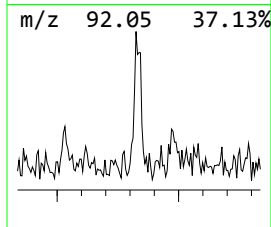
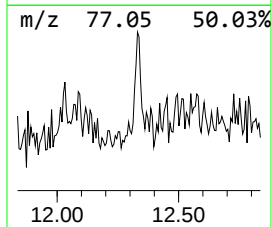
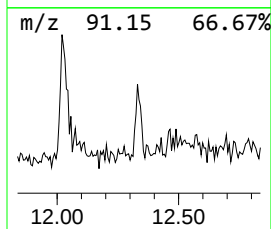
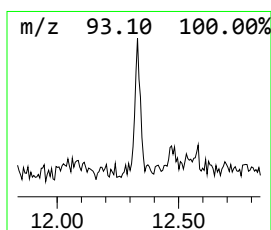
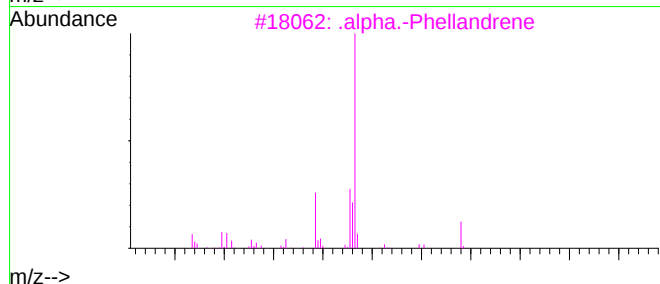
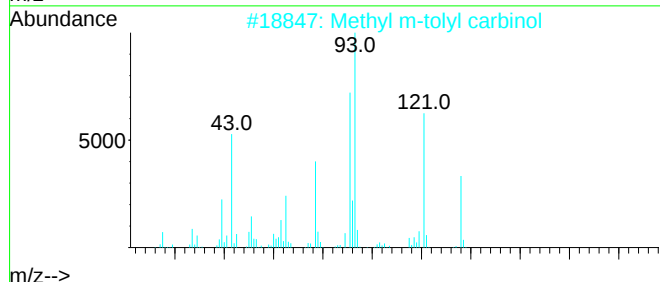
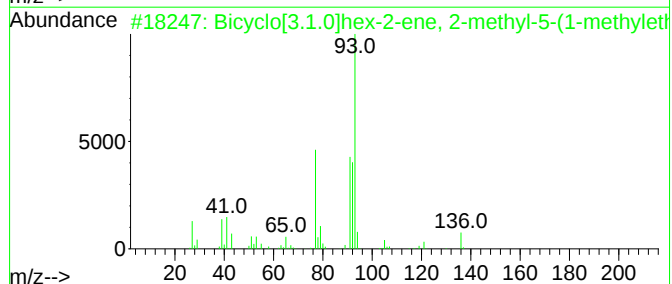
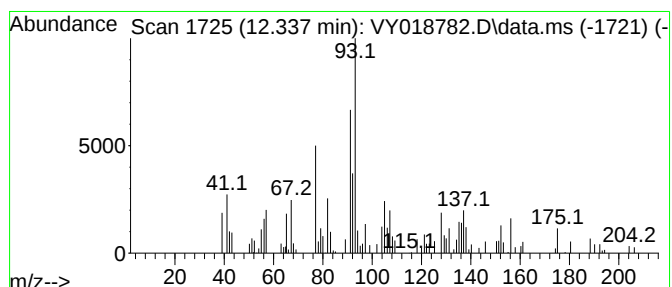
Instrument :
MSVOA_Y
ClientSampleId :
PILE-CAP

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 Bicyclo[3.1.0]hex-2-ene, 2-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.337	11.47 ug/l	22982	Chlorobenzene-d5	11.490	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.0]hex-2-ene, 2-methy...	136	C10H16	002867-05-2	52
2	Methyl m-tolyl carbinol	136	C9H12O	1010342-29-9	50
3	.alpha.-Phellandrene	136	C10H16	000099-83-2	47
4	3-Carene	136	C10H16	013466-78-9	47
5	4-Carene, (1S,3S,6R)-(-)-	136	C10H16	005208-50-4	46



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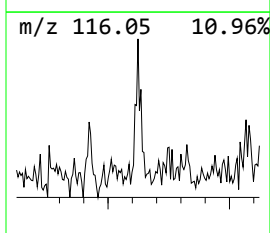
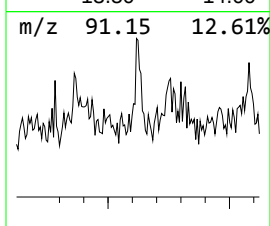
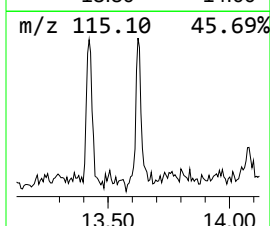
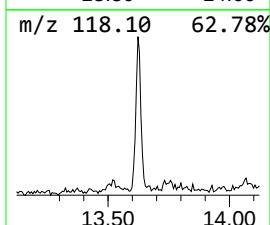
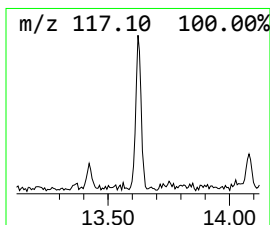
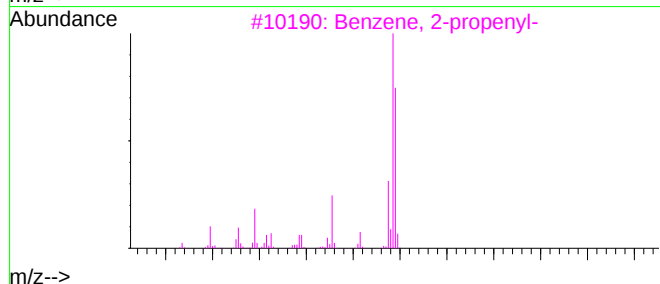
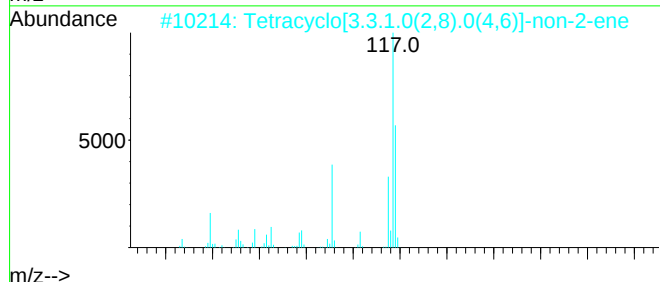
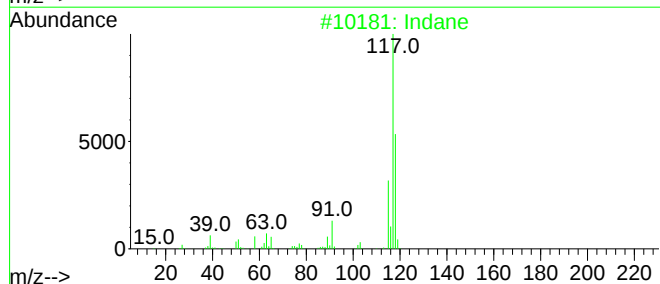
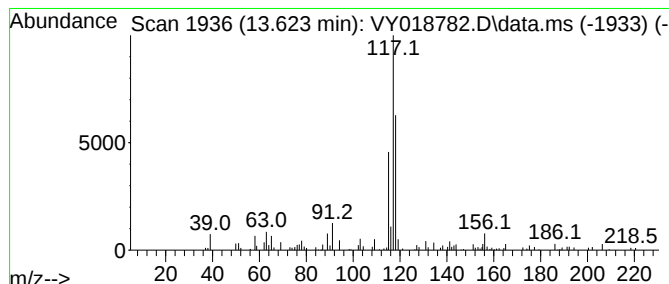
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Quant Title : SW846 8260

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

Peak Number 2 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.623	50.00 ug/l	58662	1,4-Dichlorobenzene-d4	13.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	70
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	62
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	60
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	58



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Instrument :
MSVOA_Y
ClientSampleId :
PILE-CAP

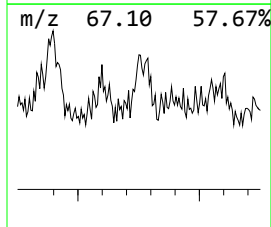
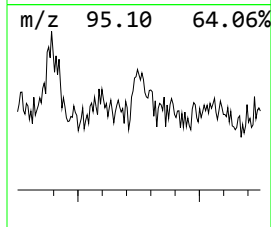
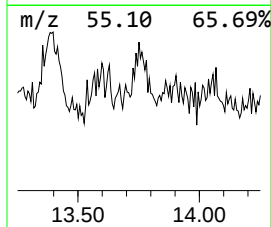
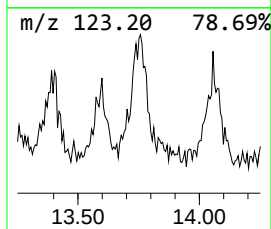
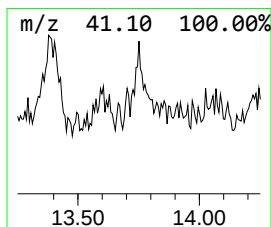
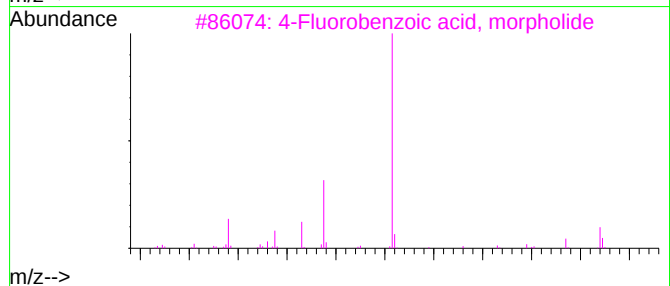
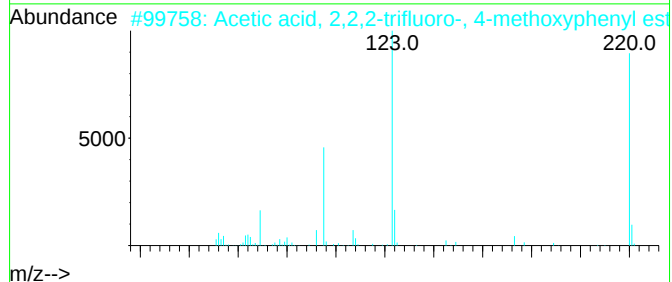
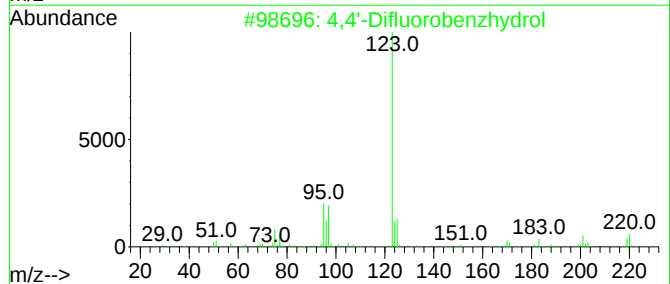
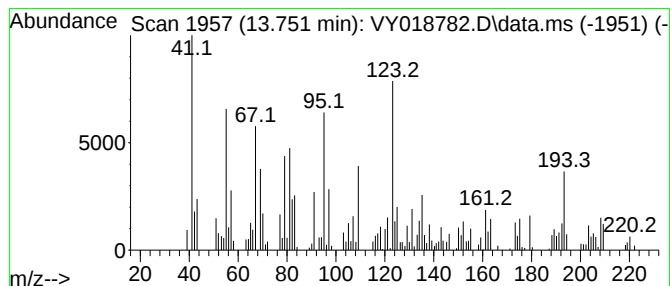
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Quant Title : SW846 8260

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

Peak Number 3 unknown13.751 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	77.87 ug/l	91364	1,4-Dichlorobenzene-d4	13.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Difluorobenzhydrol	220	C13H10F2O	000365-24-2	35
2	Acetic acid, 2,2,2-trifluoro-, 4...	220	C9H7F3O3	005672-87-7	27
3	4-Fluorobenzoic acid, morpholide	209	C11H12FNO2	1000307-09-9	27
4	2-Methylbicyclo[3.2.1]octane	124	C9H16	1010215-28-0	18
5	Dispiro[2.2.5.0]undecan-4-one, 5...	220	C15H24O	1000152-13-8	18



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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
PILE-CAP

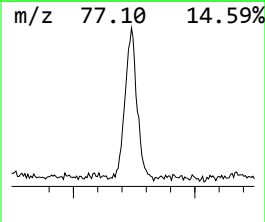
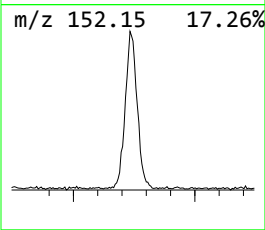
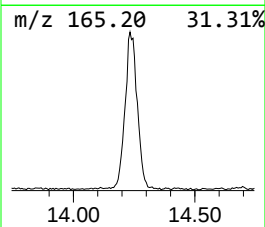
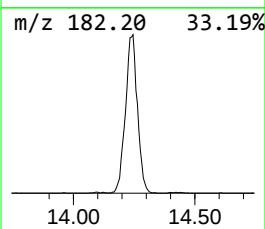
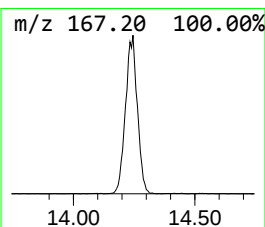
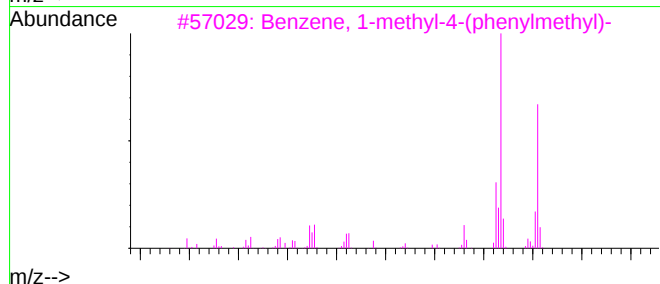
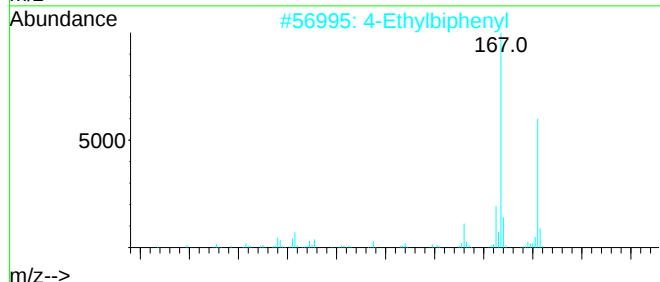
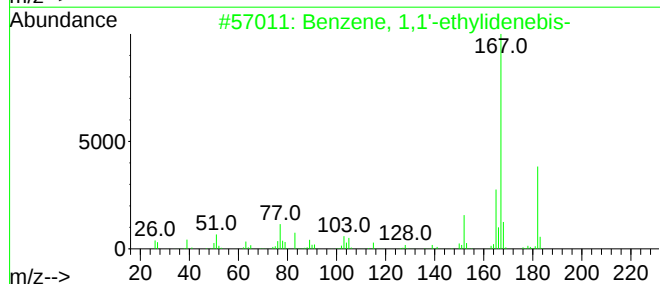
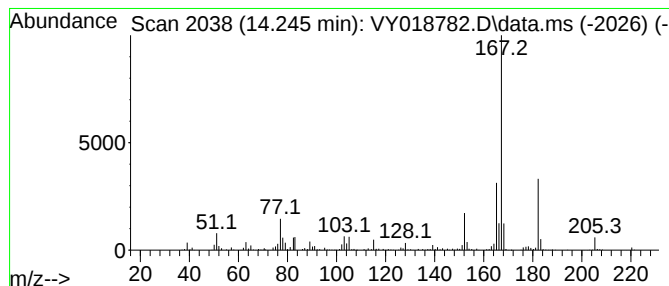
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1,1'-ethylidenebis- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.245	1038.49 ug/l	1218400	1,4-Dichlorobenzene-d4	13.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-ethylidenebis-	182	C14H14	000612-00-0	97
2	4-Ethylbiphenyl	182	C14H14	005707-44-8	90
3	Benzene, 1-methyl-4-(phenylmethyl)-	182	C14H14	000620-83-7	80
4	1,1'-Biphenyl, 4-(chloromethyl)-	202	C13H11Cl	001667-11-4	76
5	1-Benzhydryl-3-azetidinone	237	C16H15NO	040320-60-3	72



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Quant Title : SW846 8260

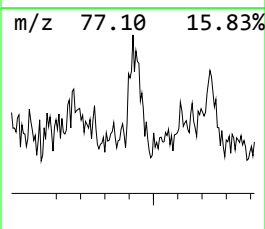
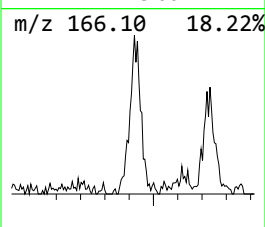
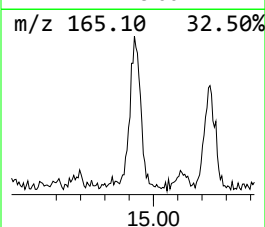
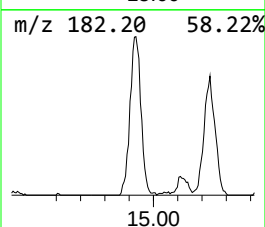
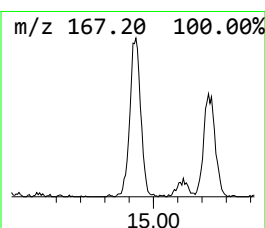
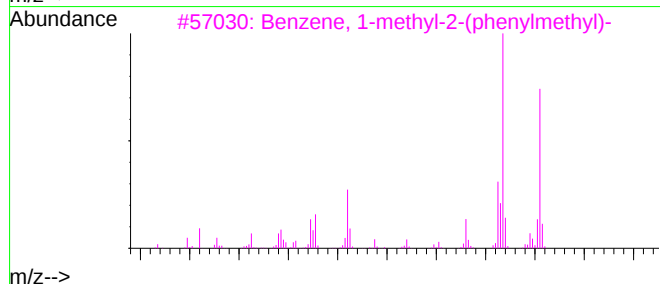
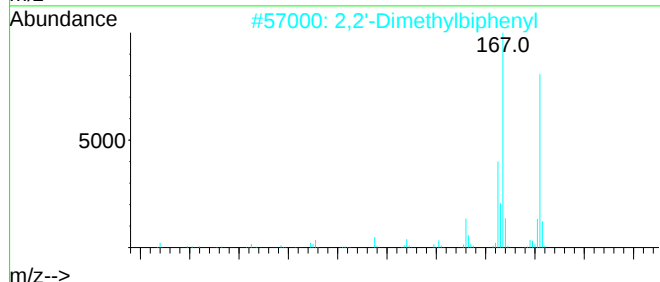
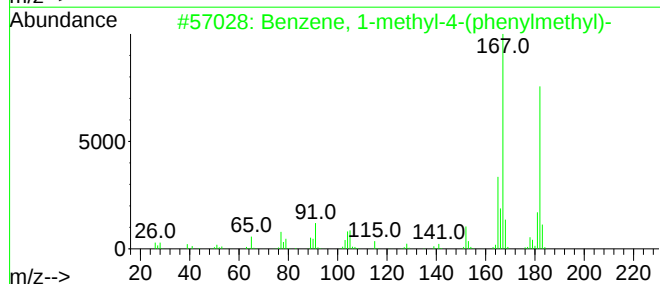
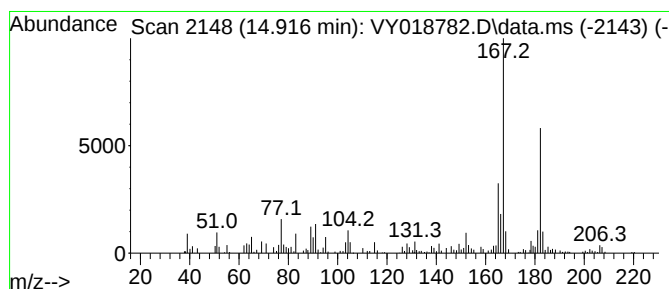
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzene, 1-methyl-4-(phenyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.916	160.91 ug/l	188780	1,4-Dichlorobenzene-d4	13.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-4-(phenylmethyl)-	182	C14H14	000620-83-7	96
2	2,2'-Dimethylbiphenyl	182	C14H14	000605-39-0	93
3	Benzene, 1-methyl-2-(phenylmethyl)-	182	C14H14	000713-36-0	93
4	Benzene, 1-methyl-3-(phenylmethyl)-	182	C14H14	000620-47-3	92
5	1,1'-Biphenyl, 2-ethyl-	182	C14H14	001812-51-7	87



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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
Bicyclo[3.1.0]h...	12.337	11.5	ug/l	22982	3	11.490	100223	50.0
Indane	13.623	50.0	ug/l	58662	4	13.422	58662	50.0
unknown13.751	13.751	77.9	ug/l	91364	4	13.422	58662	50.0
Benzene, 1,1'-e...	14.245	1038.5	ug/l	1218400	4	13.422	58662	50.0
Benzene, 1-meth...	14.916	160.9	ug/l	188780	4	13.422	58662	50.0