

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051724\
 Data File : VY018308.D
 Acq On : 17 May 2024 15:10
 Operator : SY/MD
 Sample : P2496-03
 Misc : 5.06g/5.0mL/MSVOA_Y/SOIL/B
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 CHRT-28452

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\82Y050724S.M
 Title : SW846 8260

Signal : TIC: VY018308.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	59	64	69	rBV2	8190	14461	1.81%	0.290%
2	3.058	201	203	212	rVB6	5036	11464	1.44%	0.230%
3	4.710	466	474	483	rVB4	8183	23153	2.90%	0.464%
4	5.740	632	643	651	rBV5	6571	21228	2.66%	0.425%
5	6.978	834	846	857	rBV2	6024	23026	2.89%	0.461%
6	7.709	955	966	972	rBV	110048	266597	33.41%	5.341%
7	7.783	972	978	990	rVB	182180	410538	51.45%	8.224%
8	8.136	1027	1036	1047	rBV2	97822	224062	28.08%	4.489%
9	8.685	1115	1126	1136	rBV	302055	602395	75.50%	12.068%
10	10.179	1363	1371	1378	rBV	457344	797925	100.00%	15.985%
11	11.489	1579	1586	1600	rVB	416937	685151	85.87%	13.725%
12	12.337	1719	1725	1732	rVB	140595	232022	29.08%	4.648%
13	12.483	1742	1749	1756	rBV	289457	462041	57.91%	9.256%
14	12.806	1798	1802	1805	rBV6	8084	13054	1.64%	0.262%
15	12.891	1810	1816	1824	rVB	113839	188420	23.61%	3.775%
16	13.141	1853	1857	1862	rBV2	16830	27092	3.40%	0.543%
17	13.422	1898	1903	1911	rVB	311733	514637	64.50%	10.310%
18	13.745	1951	1956	1962	rBV8	27246	58815	7.37%	1.178%
19	14.080	2007	2011	2014	rBV6	11630	19358	2.43%	0.388%
20	14.251	2036	2039	2043	rBV3	32924	48986	6.14%	0.981%
21	14.422	2064	2067	2070	rVB4	25082	31862	3.99%	0.638%
22	14.617	2096	2099	2103	rBV5	12398	16244	2.04%	0.325%
23	14.733	2114	2118	2122	rVB5	35396	58186	7.29%	1.166%
24	14.842	2133	2136	2139	rBV4	27776	38294	4.80%	0.767%
25	14.940	2148	2152	2156	rVB6	29535	50811	6.37%	1.018%
26	15.263	2202	2205	2207	rBV3	19375	27570	3.46%	0.552%
27	15.293	2207	2210	2216	rVV5	24463	54814	6.87%	1.098%
28	15.732	2278	2282	2291	rVB9	32457	69617	8.72%	1.395%

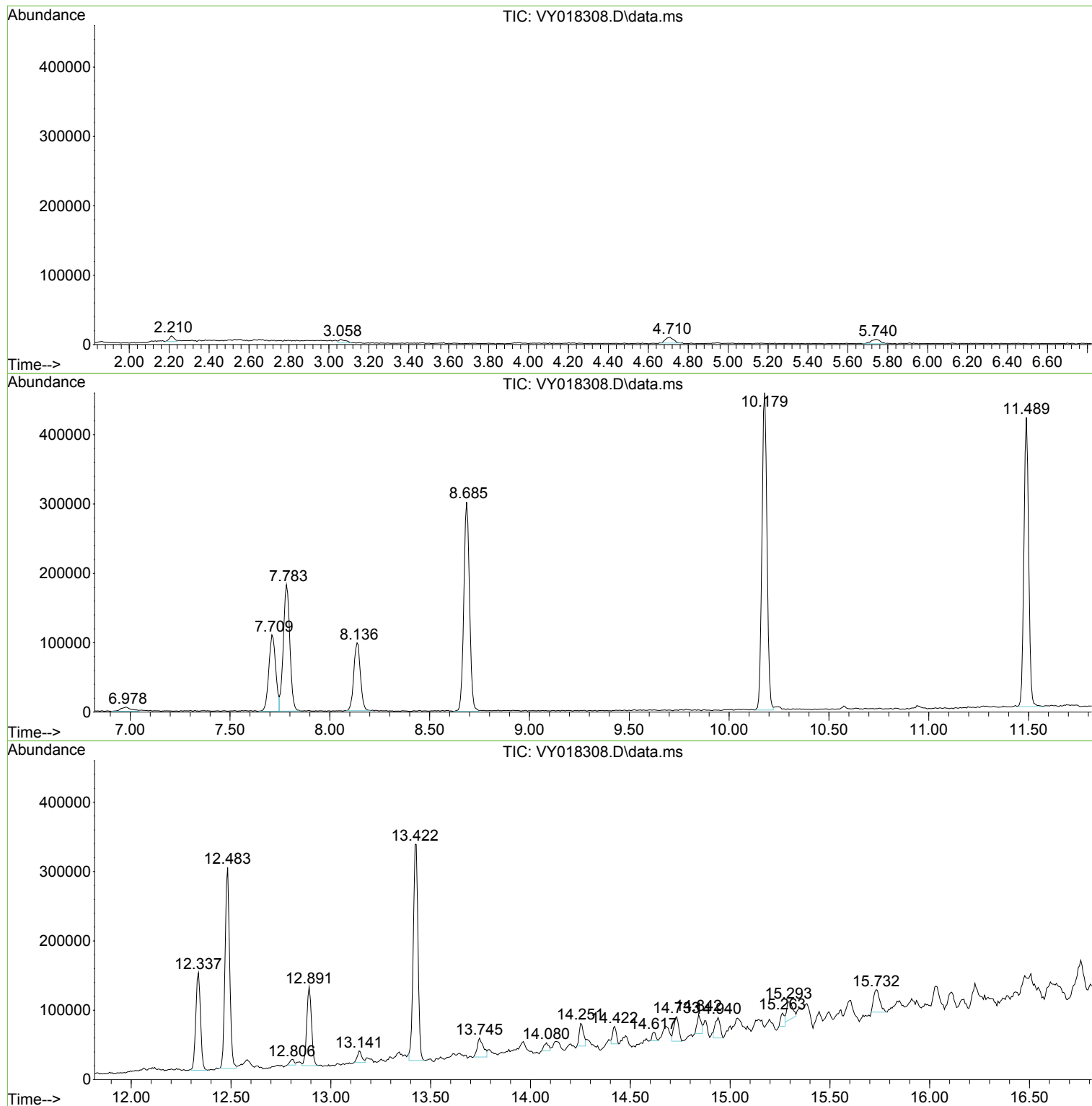
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-28452

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y050724S.M
Quant Title : SW846 8260

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



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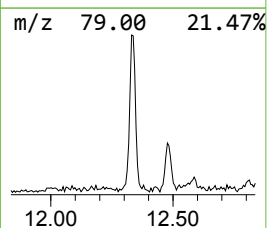
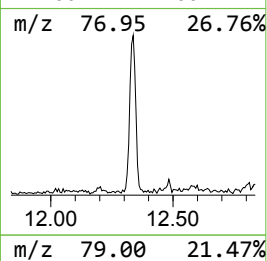
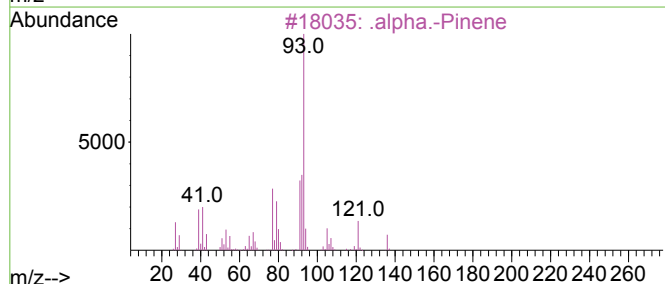
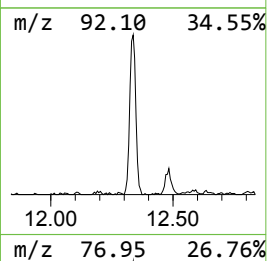
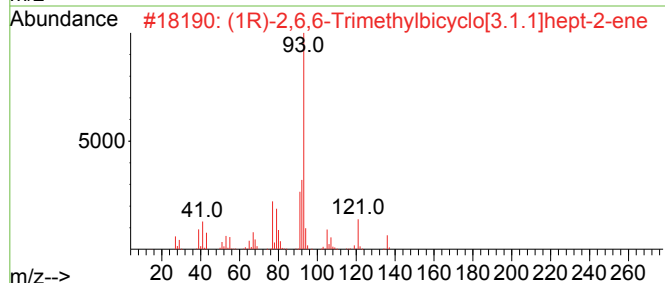
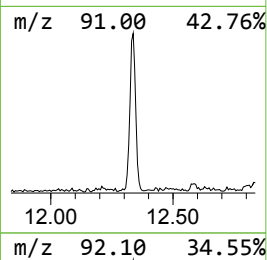
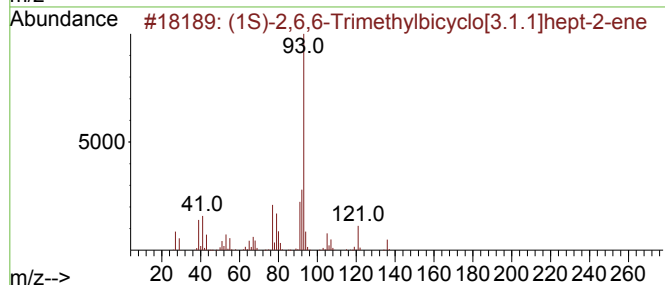
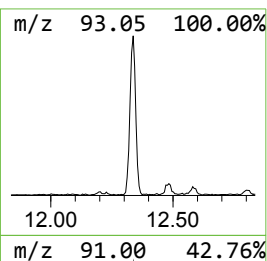
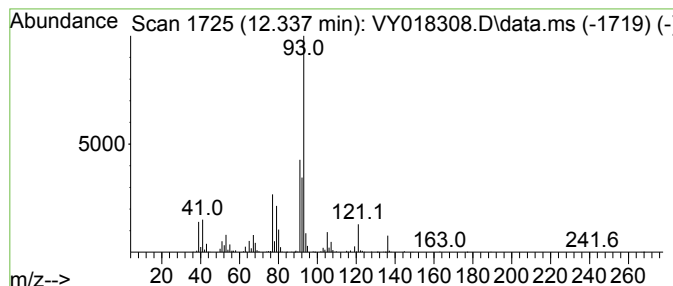
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y050724S.M
Quant Title : SW846 8260

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

Peak Number 1 (1S)-2,6,6-Trimethylbicyclo... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.337	16.93 ug/l	232022	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1S)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-26-4	97		
2	(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	97		
3	.alpha.-Pinene	136	C10H16	000080-56-8	96		
4	Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	136	C10H16	004889-83-2	95		
5	Tricyclo[2.2.1.0(2,6)]heptane, 1,1,2-trimethyl-	136	C10H16	000508-32-7	91		



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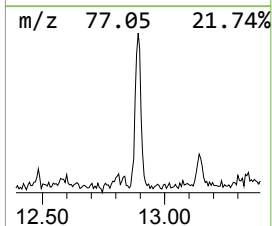
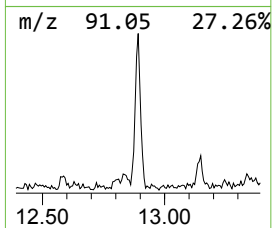
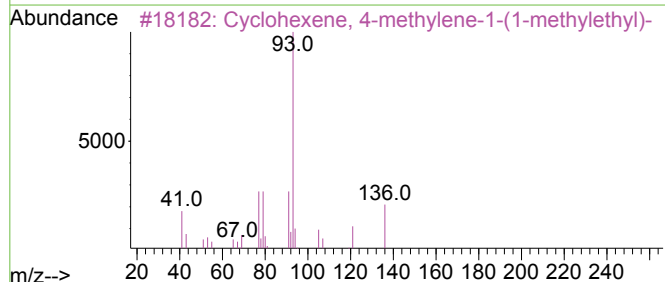
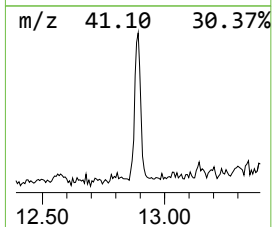
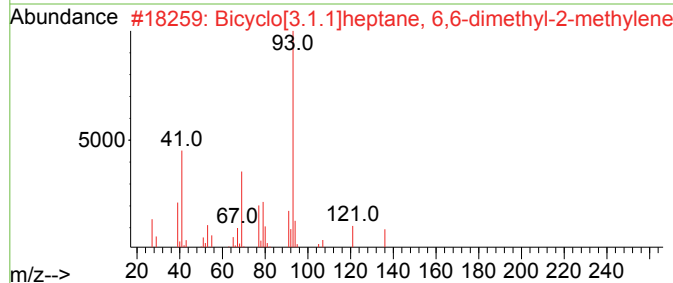
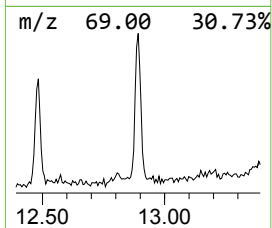
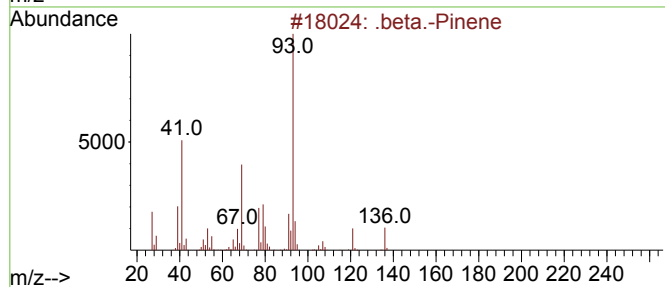
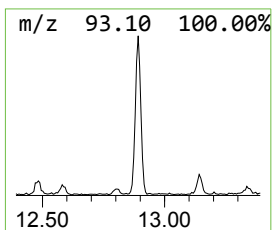
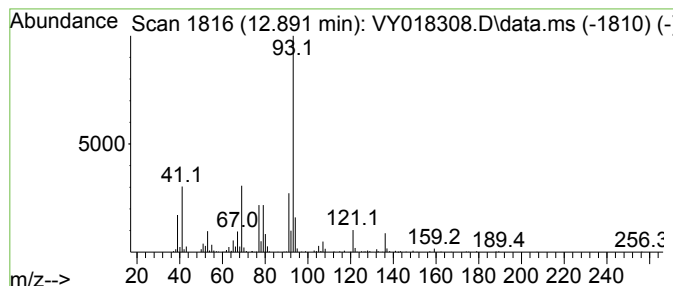
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y050724S.M
Quant Title : SW846 8260

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

Peak Number 2 .beta.-Pinene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.892	18.31 ug/l	188420	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.beta.-Pinene	136	C10H16	000127-91-3	94
2			Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	91
3			Cyclohexene, 4-methylene-1-(1-me...	136	C10H16	000099-84-3	91
4			Cyclohexane, 1-methylene-4-(1-me...	136	C10H16	000499-97-8	90
5			Bicyclo[3.1.0]hexane, 4-methylen...	136	C10H16	003387-41-5	87



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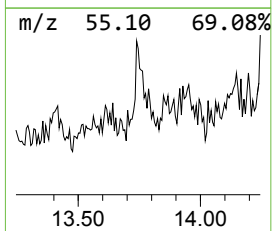
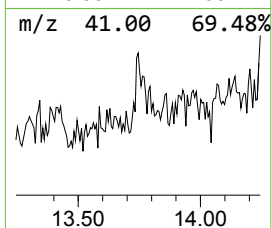
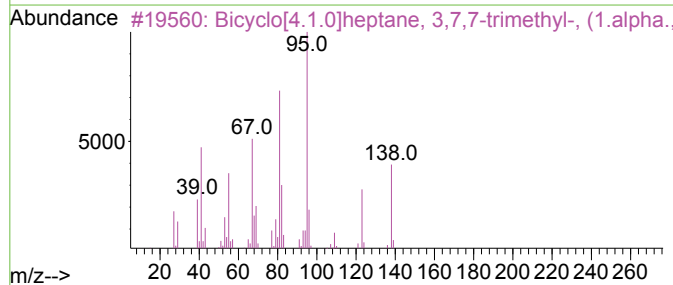
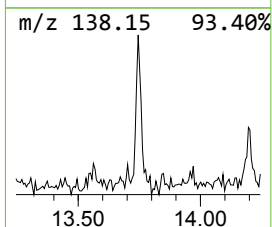
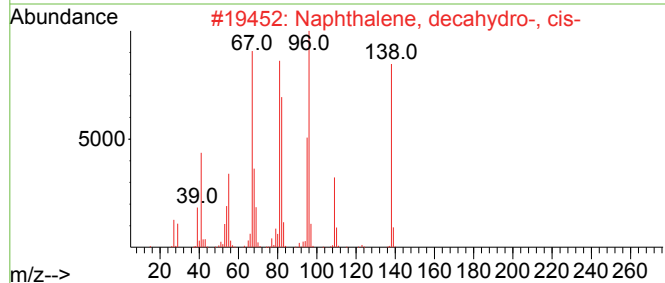
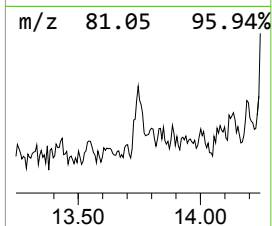
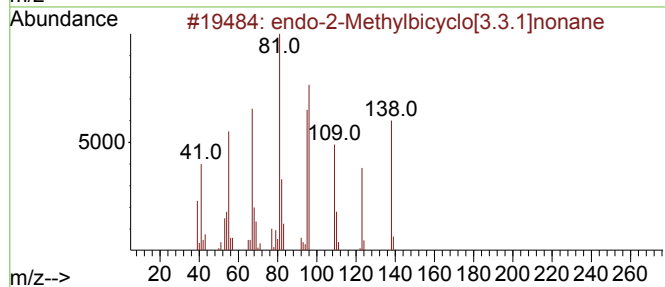
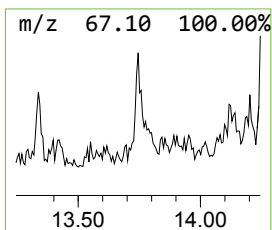
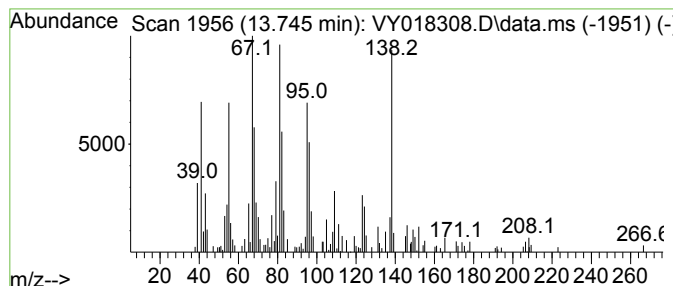
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y050724S.M
Quant Title : SW846 8260

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

Peak Number 3 endo-2-Methylbicyclo[3.3.1]... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.745	5.71 ug/l	58815	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			endo-2-Methylbicyclo[3.3.1]nonane	138	C10H18	042558-37-2	87
2			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	81
3			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	018968-23-5	81
4			4-Isopropenylcyclohexanone	138	C9H14O	022460-53-3	76
5			Cyclodecene	138	C10H18	003618-12-0	74



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Instrument :
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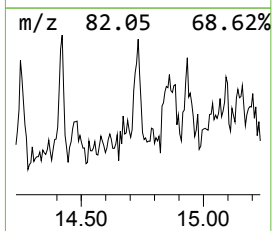
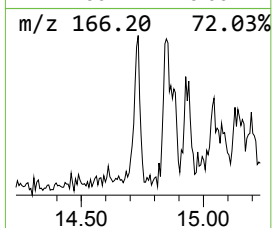
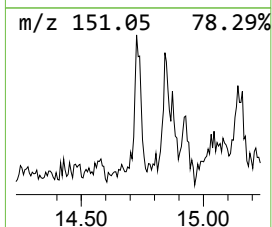
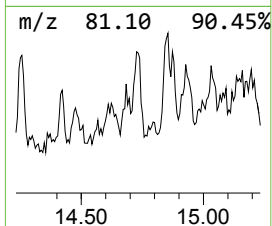
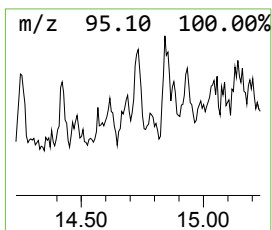
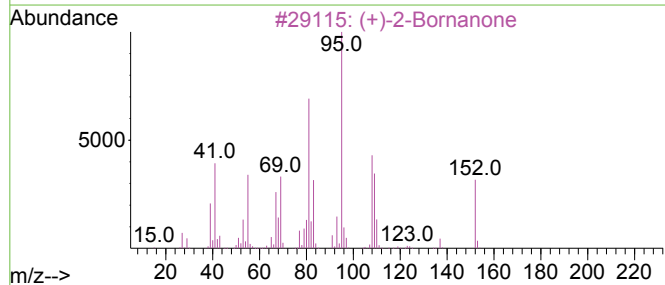
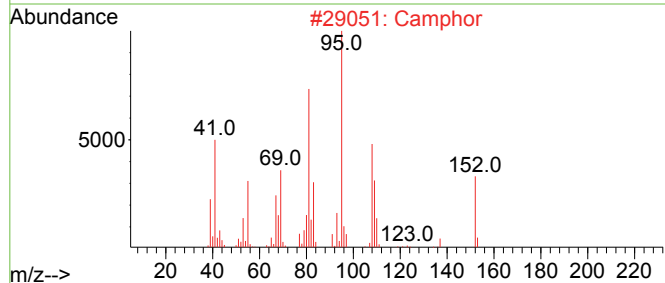
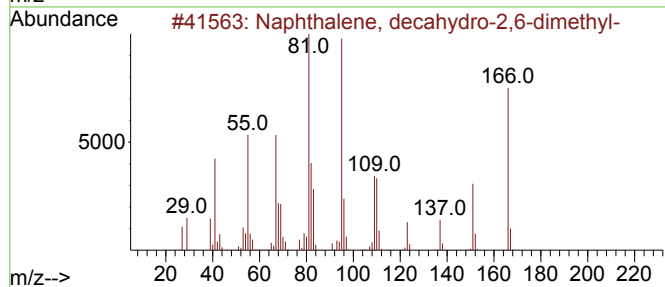
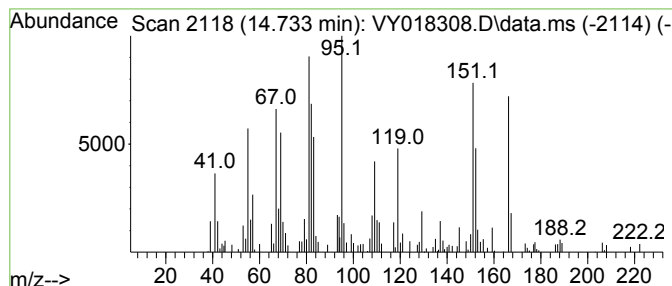
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Peak Number 4 Naphthalene, decahydro-2,6-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.733	5.65 ug/l	58186	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	53
2			Camphor	152	C10H16O	000076-22-2	50
3			(+)-2-Bornanone	152	C10H16O	000464-49-3	50
4			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	50
5			trans,trans-1,6-Dimethylspiro[4...	166	C12H22	1000111-72-1	50



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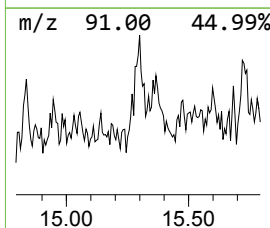
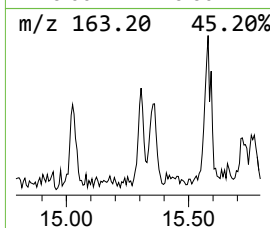
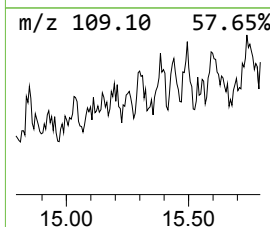
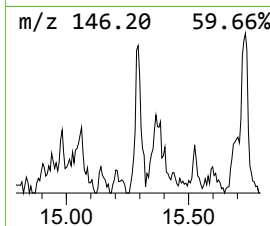
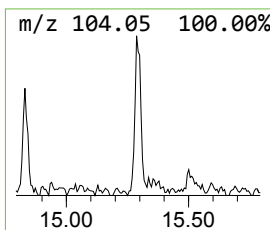
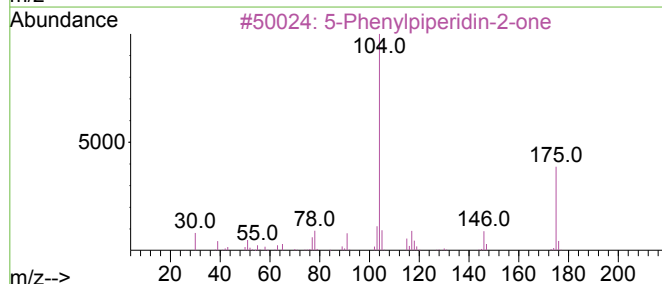
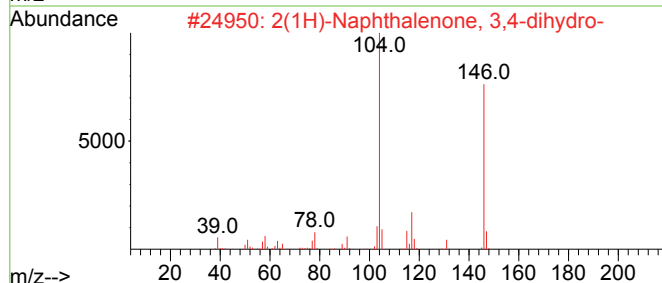
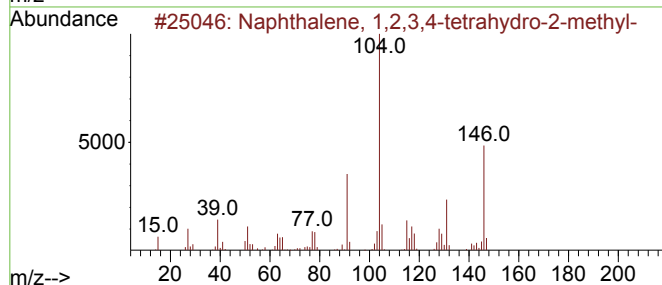
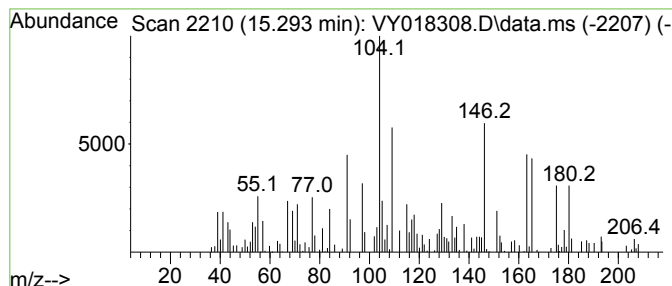
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y050724S.M
Quant Title : SW846 8260

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

Peak Number 5 unknown15.294 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.294	5.33 ug/l	54814	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	003877-19-8	30
2			2(1H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000530-93-8	22
3			5-Phenylpiperidin-2-one	175	C11H13NO	003973-63-5	18
4			1H-1,2,3-benzotriazole, 6-butyl-	175	C10H13N3	1000404-71-0	14
5			Isoxazole, 3-ethyl-4,5-dihydro-5...	175	C11H13NO	1000362-14-9	14



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CHRT-28452

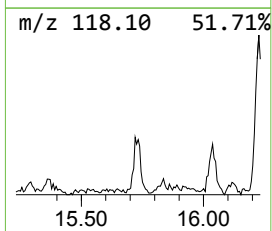
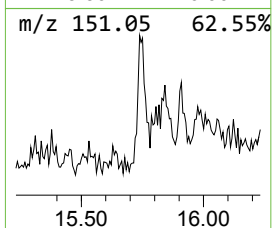
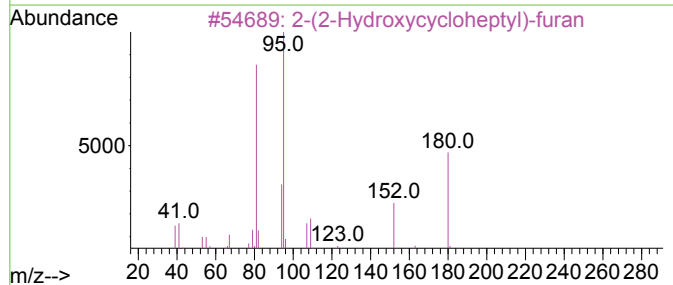
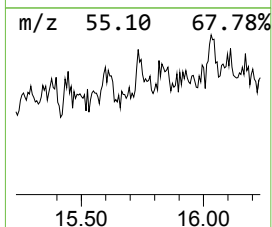
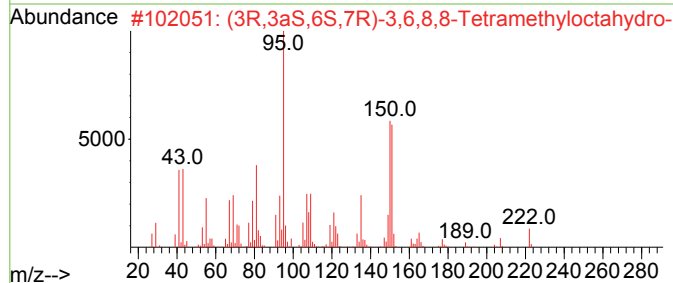
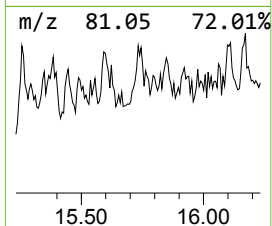
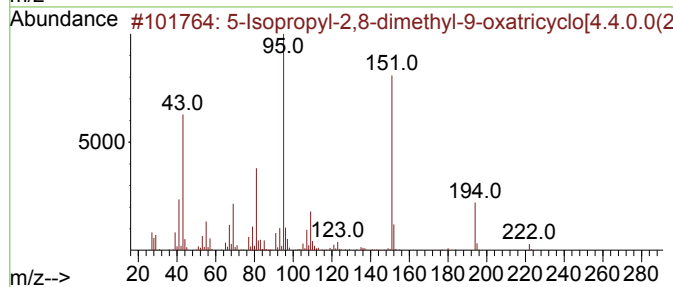
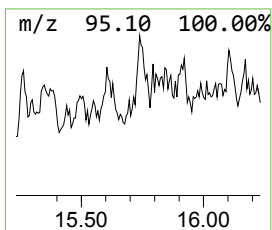
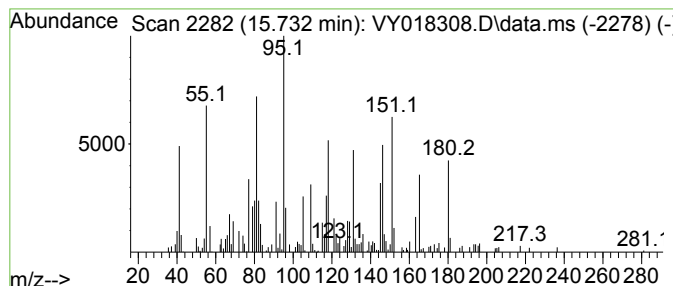
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y050724S.M
Quant Title : SW846 8260

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

Peak Number 6 unknown15.732 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.732	6.76 ug/l	69617	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Isopropyl-2,8-dimethyl-9-oxatr...	222	C14H22O2	1010185-23-8	30		
2	(3R,3aS,6S,7R)-3,6,8,8-Tetrameth...	222	C15H26O	019903-73-2	22		
3	2-(2-Hydroxycycloheptyl)-furan	180	C11H16O2	1000145-02-9	22		
4	1,4-Benzodioxan-6-amine	151	C8H9NO2	022013-33-8	18		
5	Bicyclo[2.2.1]heptane, 2-butyl-	152	C11H20	061177-16-0	15		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051724\
Data File : VY018308.D
Acq On : 17 May 2024 15:10
Operator : SY/MD
Sample : P2496-03
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-28452

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y050724S.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
(1S)-2,6,6-Trim...	12.337	16.9	ug/l	232022	3	11.489	685151	50.0
.beta.-Pinene	12.892	18.3	ug/l	188420	4	13.428	514637	50.0
endo-2-Methylbi...	13.745	5.7	ug/l	58815	4	13.428	514637	50.0
Naphthalene, de...	14.733	5.7	ug/l	58186	4	13.428	514637	50.0
unknown15.294	15.294	5.3	ug/l	54814	4	13.428	514637	50.0
unknown15.732	15.732	6.8	ug/l	69617	4	13.428	514637	50.0