

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD051923\
 Data File : VD076163.D
 Acq On : 19 May 2023 18:39
 Operator : KP/SY
 Sample : 02849-11
 Misc : 4.92G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 TP8

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_D\Method\82D051523S.M
 Title : SW846 8260

Signal : TIC: VD076163.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.728	18	24	34	rBV	261272	462385	34.24%	18.242%
2	7.804	1052	1057	1064	rBV4	7556	16506	1.22%	0.651%
3	8.228	1122	1129	1136	rBV2	8664	18642	1.38%	0.735%
4	8.775	1215	1222	1230	rVB2	12136	24152	1.79%	0.953%
5	10.269	1468	1476	1483	rBV	18552	32045	2.37%	1.264%
6	11.581	1693	1699	1707	rVB	20013	35142	2.60%	1.386%
7	12.398	1814	1838	1863	rBV8	210039	1350406	100.00%	53.277%
8	12.575	1863	1868	1877	rVB2	25101	47285	3.50%	1.866%
9	13.516	2013	2028	2034	rBV3	38516	94677	7.01%	3.735%
10	13.904	2081	2094	2103	rBV8	17042	66897	4.95%	2.639%
11	14.022	2103	2114	2115	rBV6	26633	55581	4.12%	2.193%
12	14.457	2174	2188	2204	rVB7	56123	260647	19.30%	10.283%
13	14.657	2214	2222	2229	rVB7	8392	19799	1.47%	0.781%
14	14.775	2234	2242	2245	rVV3	8084	17963	1.33%	0.709%
15	14.839	2247	2253	2255	rVV7	7879	18986	1.41%	0.749%
16	14.892	2261	2262	2269	rVB3	12052	13574	1.01%	0.536%

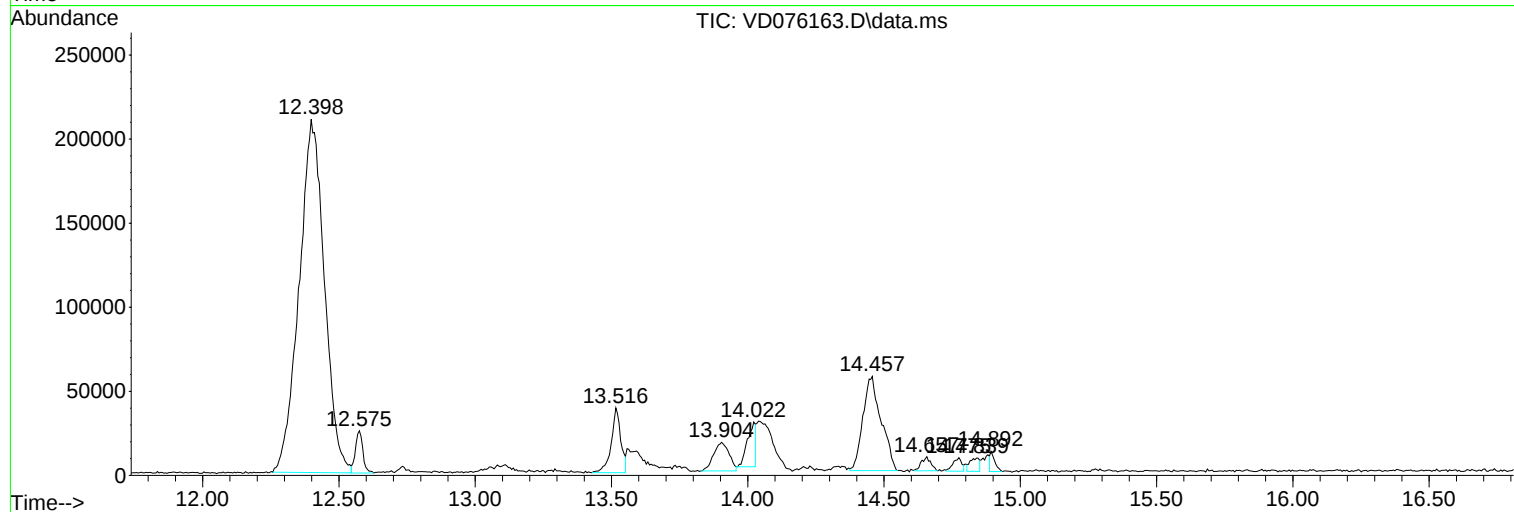
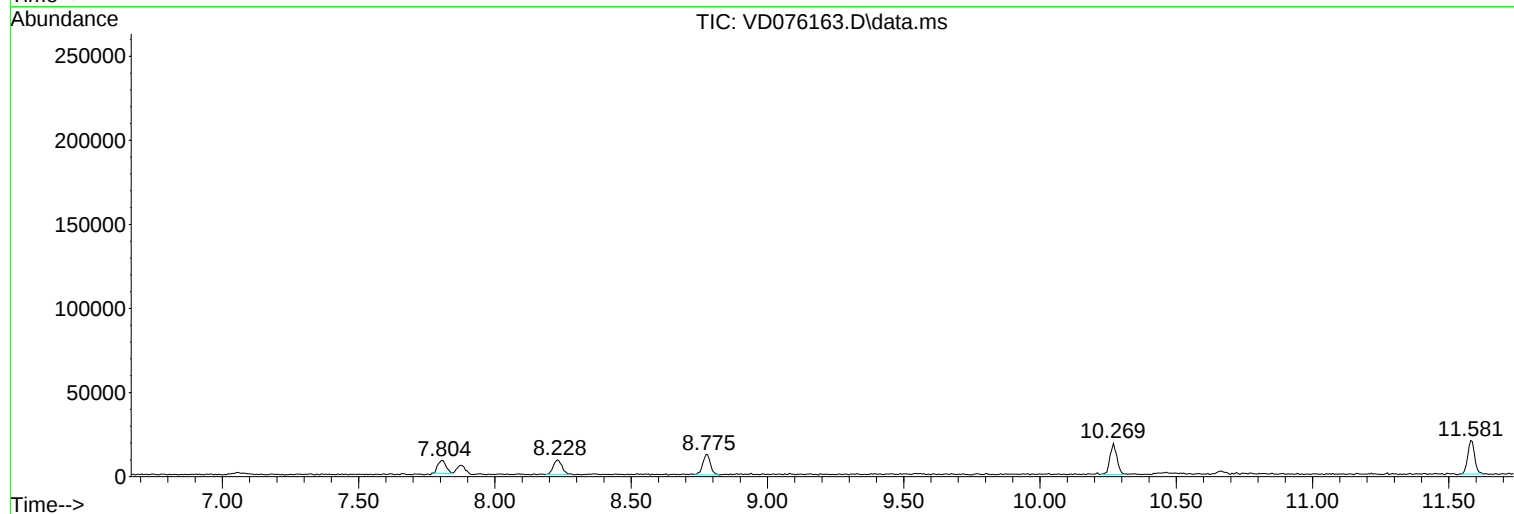
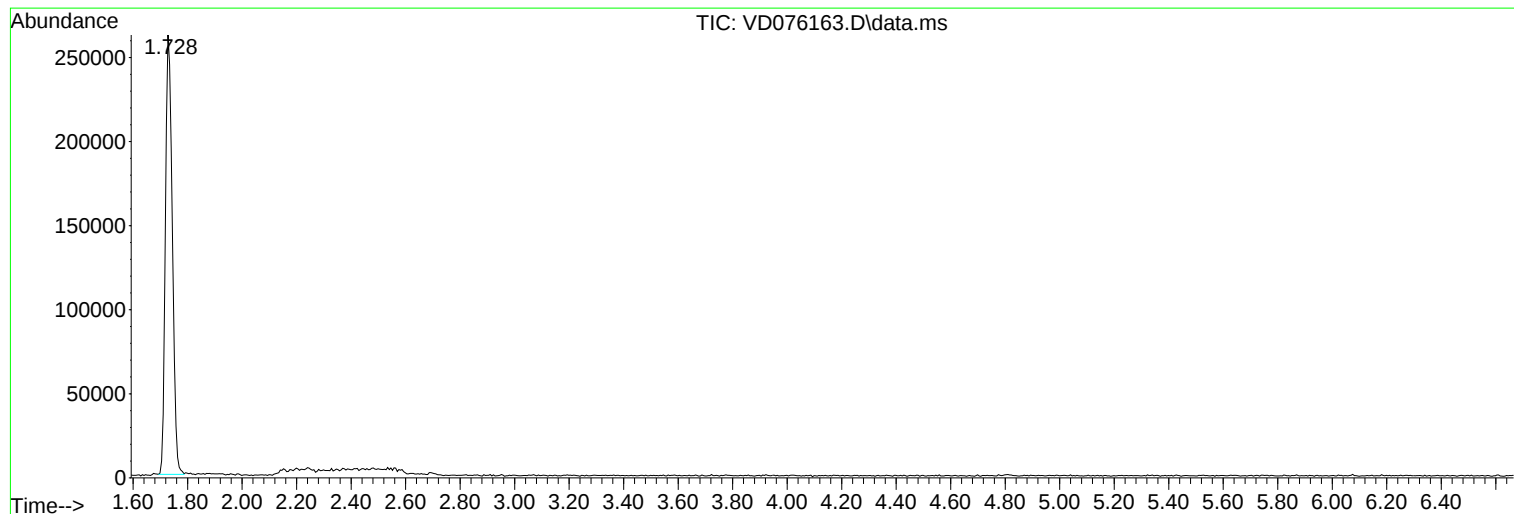
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D051523S.M
Quant Title : SW846 8260

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



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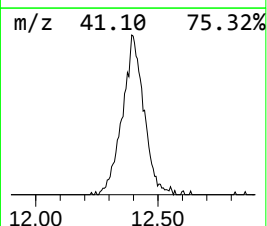
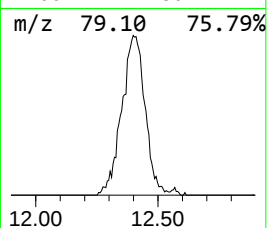
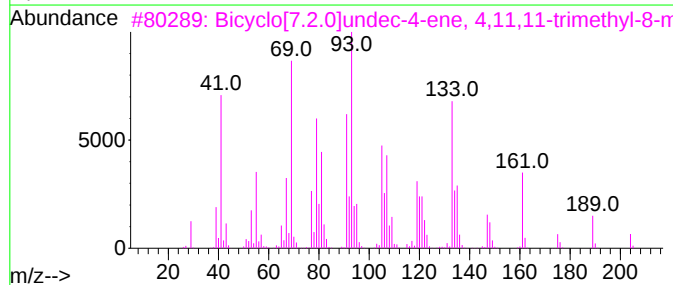
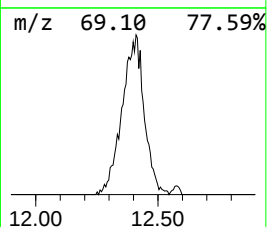
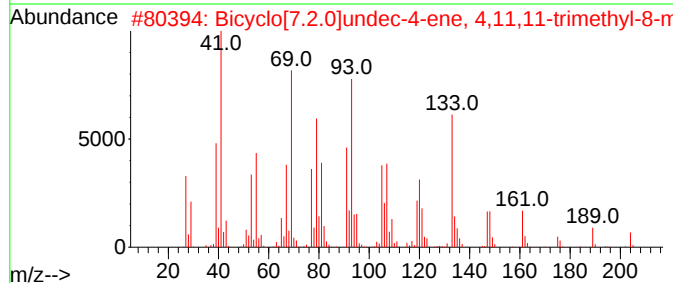
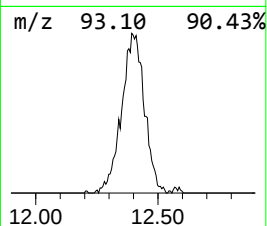
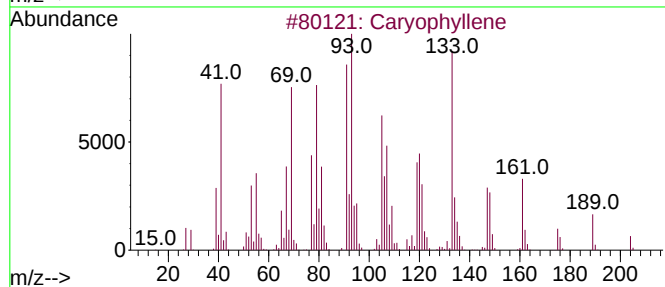
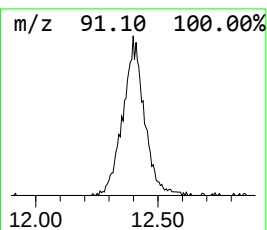
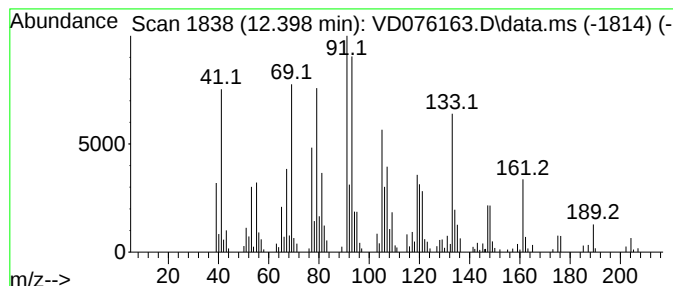
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D051523S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Caryophyllene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.398	1921.36 ug/l	1350410	Chlorobenzene-d5	11.581

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Caryophyllene	204	C15H24	000087-44-5	99
2			Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	97
3			Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	93
4			Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	60
5			Cyclohexene, 5-methyl-3-(1-methy...	136	C10H16	056816-08-1	46



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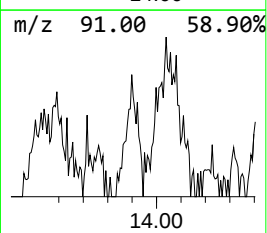
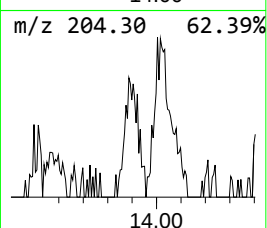
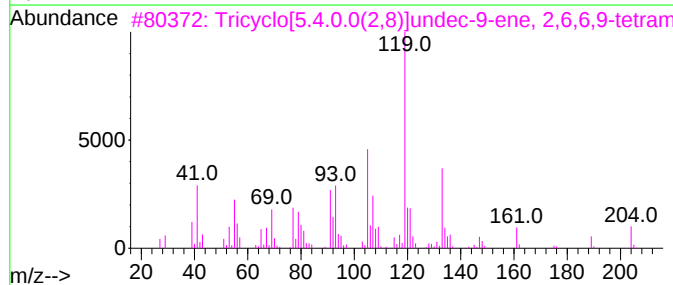
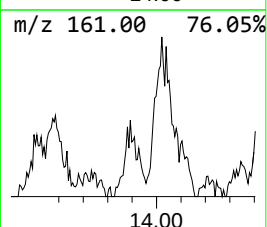
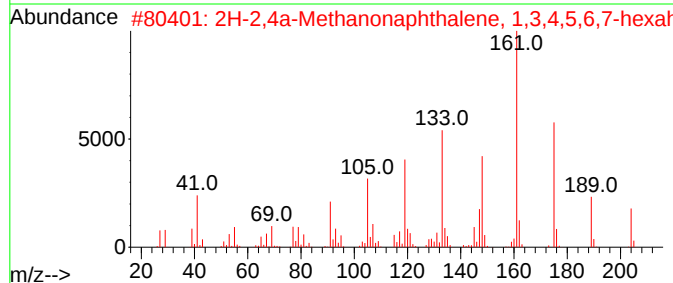
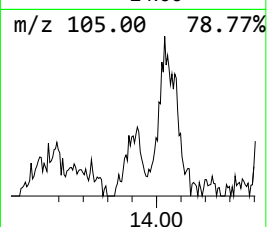
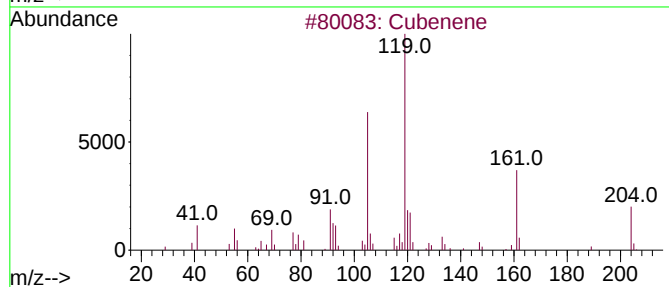
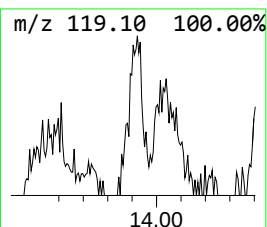
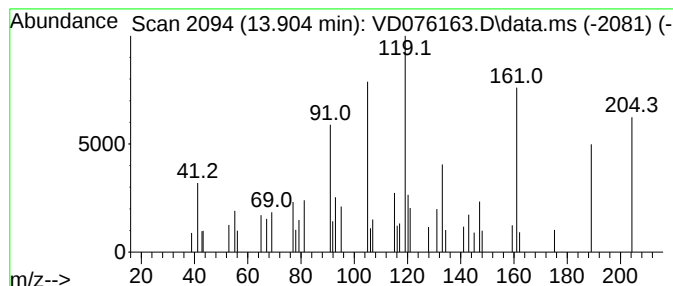
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D051523S.M
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Peak Number 3 Cubenene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	35.33 ug/l	66897	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cubenene	204	C15H24	029837-12-5	60
2			2H-2,4a-Methanonaphthalene, 1,3,...	204	C15H24	001135-66-6	58
3			Tricyclo[5.4.0.0(2,8)]undec-9-en...	204	C15H24	005989-08-2	55
4			Naphthalene, 1,2,3,4,4a,7-hexahy...	204	C15H24	016728-99-7	53
5			Acetonitrile, (3,5,5-trimethyl-2...	161	C11H15N	069697-21-8	49



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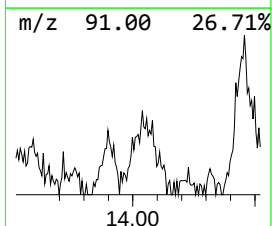
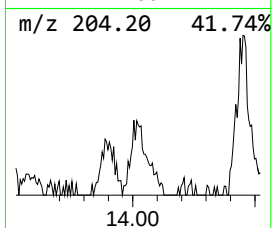
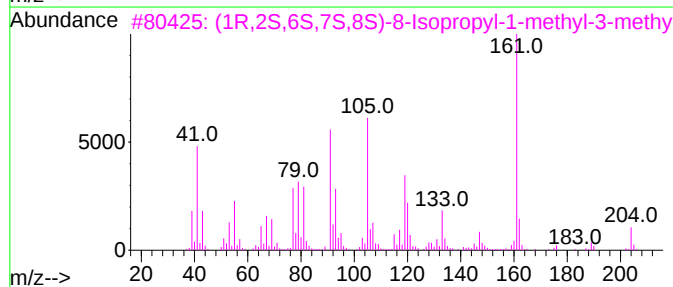
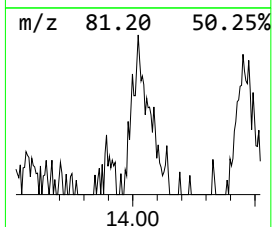
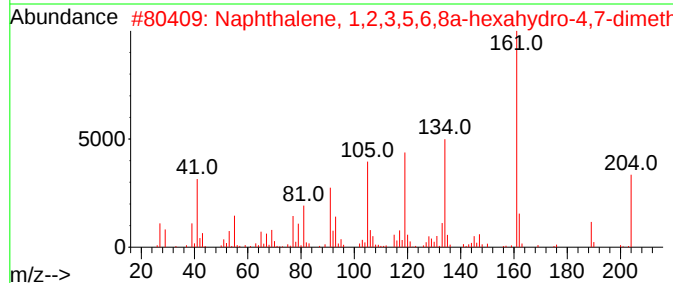
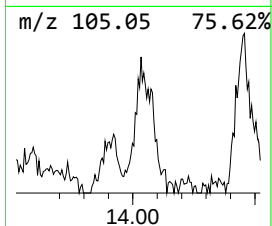
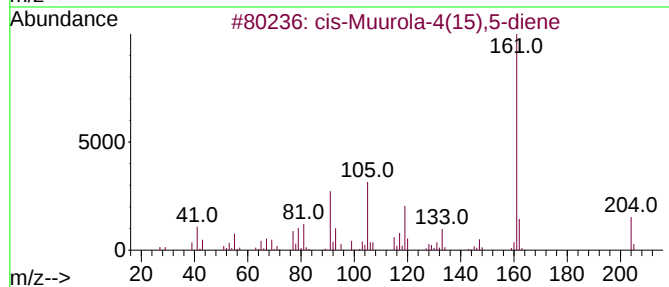
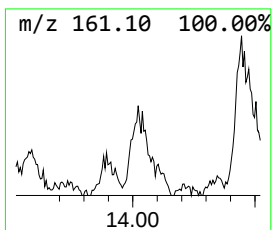
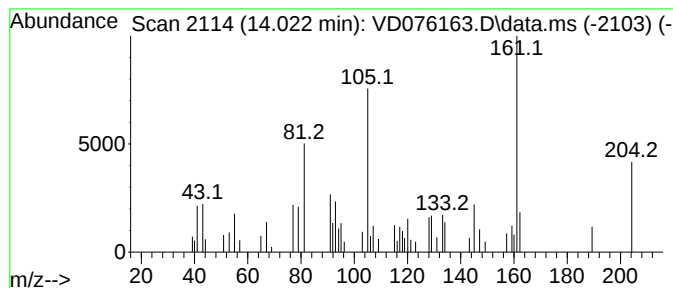
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 cis-Muurola-4(15),5-diene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.022	29.35 ug/l	55581	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Muurola-4(15),5-diene	204	C15H24	157477-72-0	86
2			Naphthalene, 1,2,3,5,6,8a-hexahy...	204	C15H24	000483-76-1	72
3			(1R,2S,6S,7S,8S)-8-Isopropyl-1-m...	204	C15H24	018252-44-3	64
4			(+)-epi-Bicyclosquiphellandrene	204	C15H24	054274-73-6	62
5			Germacrene D	204	C15H24	023986-74-5	53



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ALS Vial : 18 Sample Multiplier: 1

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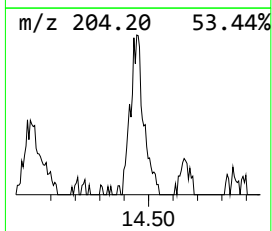
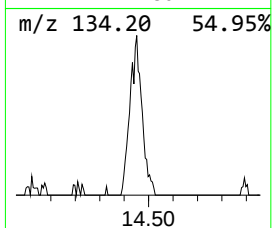
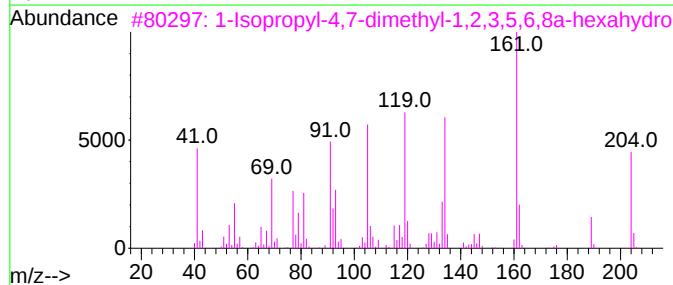
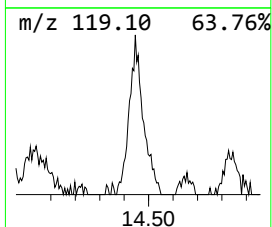
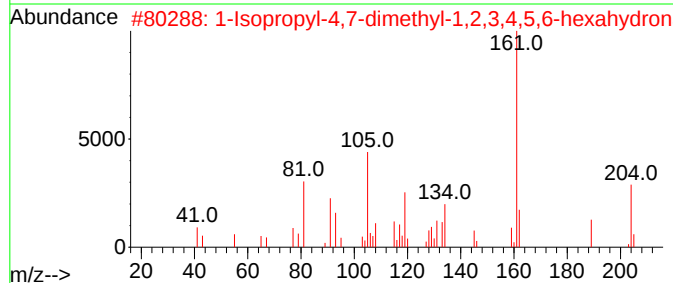
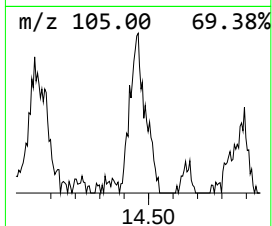
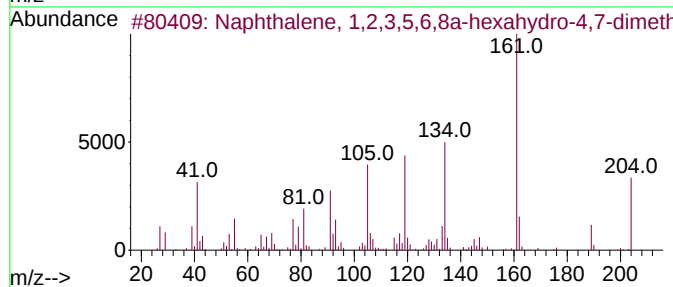
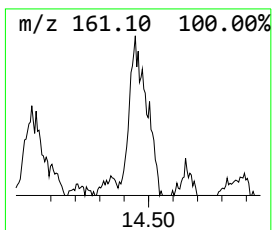
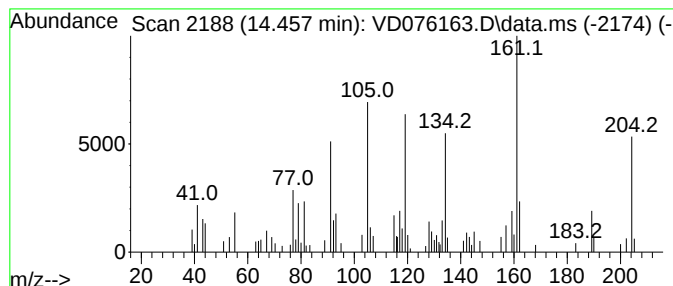
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Naphthalene, 1,2,3,5,6,8a-h... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.457	137.65 ug/l	260647	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,5,6,8a-hexahy...	204	C15H24	000483-76-1	95
2			1-Isopropyl-4,7-dimethyl-1,2,3,4...	204	C15H24	016729-00-3	91
3			1-Isopropyl-4,7-dimethyl-1,2,3,5...	204	C15H24	016729-01-4	81
4			2,6-Dimethyl-1,3,5,7-octatetraen...	134	C10H14	000460-01-5	70
5			Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	000523-47-7	55



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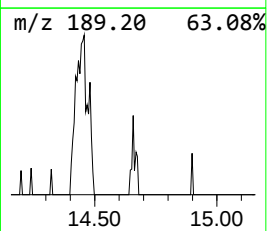
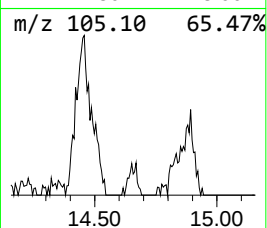
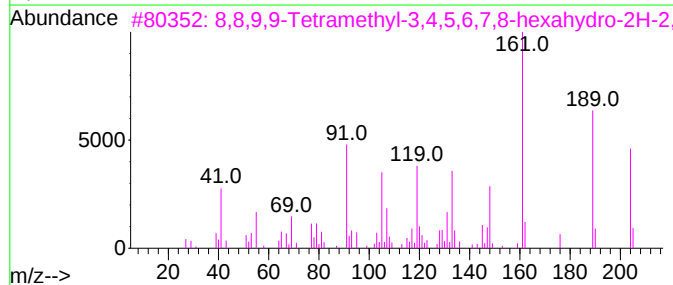
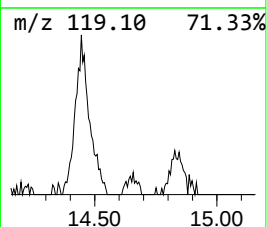
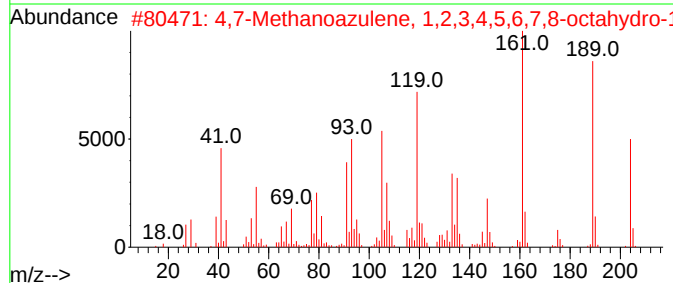
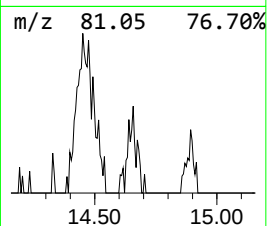
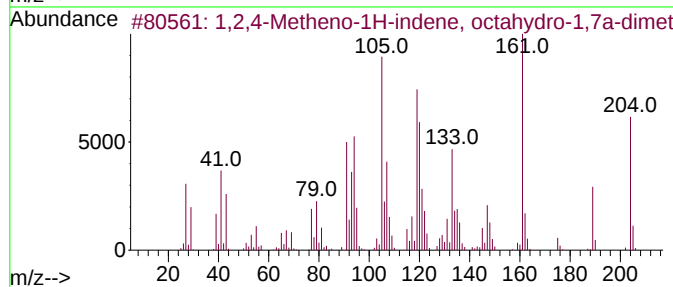
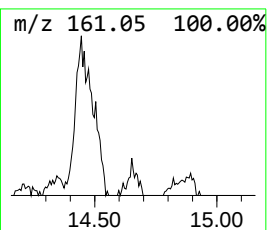
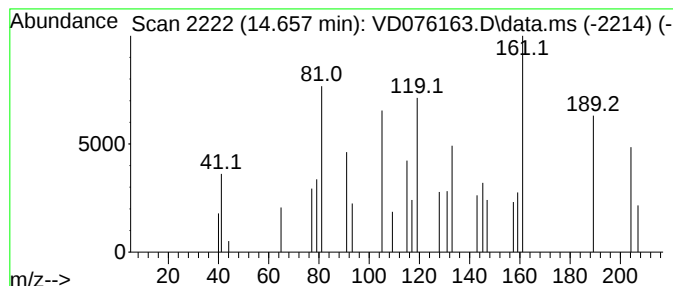
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 unknown14.657 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.657	10.46 ug/l	19799	1,4-Dichlorobenzene-d4	13.516	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Metheno-1H-indene, octahyd...	204	C15H24	022469-52-9	49
2	4,7-Methanoazulene, 1,2,3,4,5,6,...	204	C15H24	000514-51-2	49
3	8,8,9,9-Tetramethyl-3,4,5,6,7,8-...	204	C15H24	026783-22-2	47
4	isolekene	204	C15H24	095910-36-4	47
5	(-)-Aristolene	204	C15H24	006831-16-9	47



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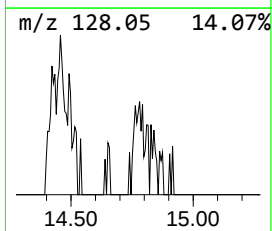
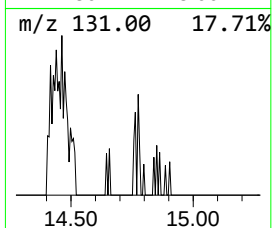
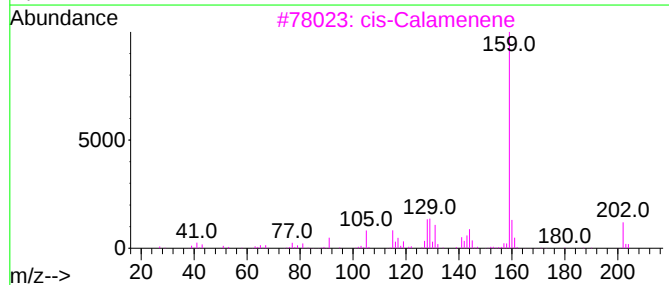
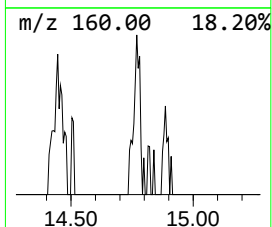
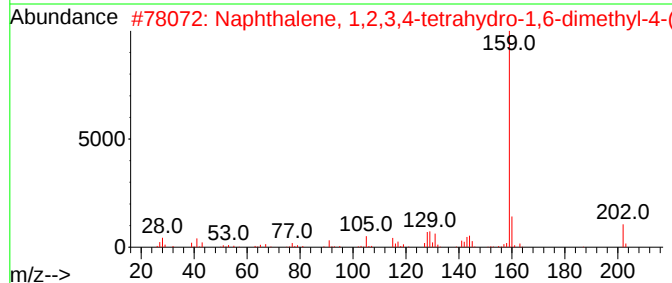
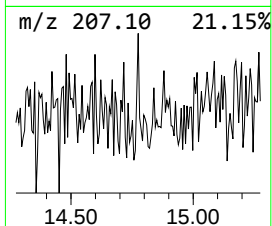
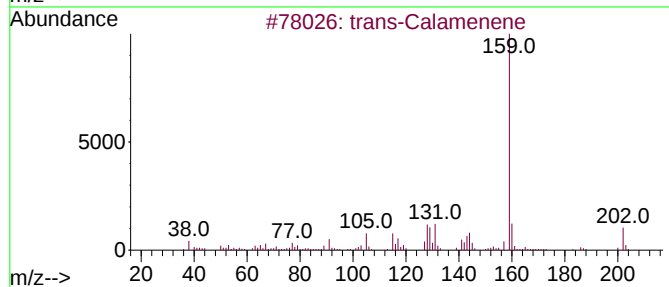
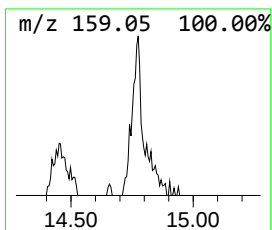
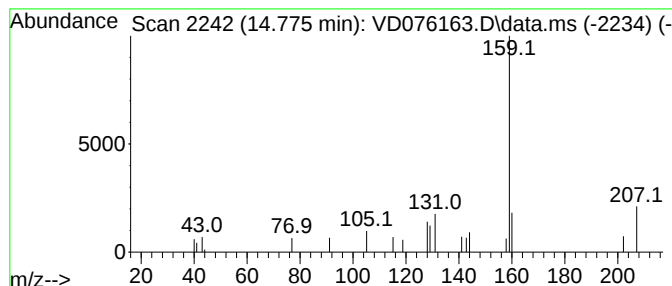
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Quant Title : SW846 8260

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

Peak Number 7 trans-Calamenene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.775	9.49 ug/l	17963	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Calamenene	202	C15H22	073209-42-4	83
2			Naphthalene, 1,2,3,4-tetrahydro-...	202	C15H22	000483-77-2	80
3			cis-Calamenene	202	C15H22	072937-55-4	80
4			Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	000475-03-6	64
5			4-isopropyl-1,6-dimethyl-1,2,3,4-...	202	C15H22	1000378-99-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD051923\
Data File : VD076163.D
Acq On : 19 May 2023 18:39
Operator : KP/SY
Sample : 02849-11
Misc : 4.92G/5.00ml/MSVOA_D/SOIL
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
TP8

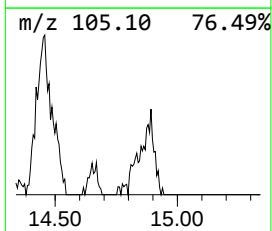
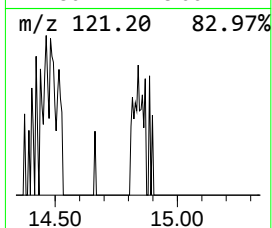
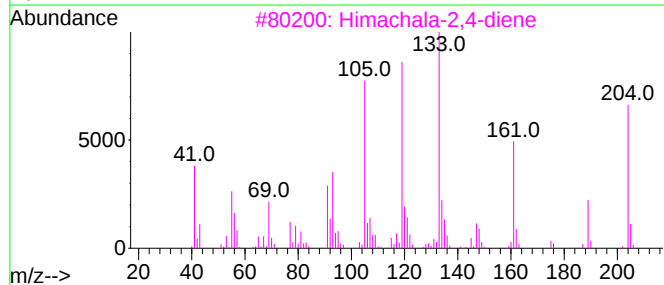
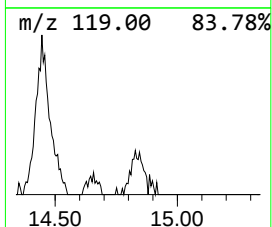
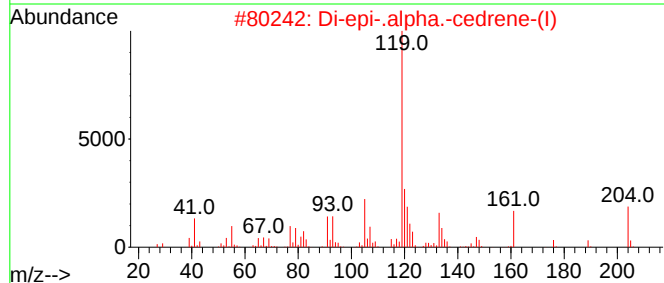
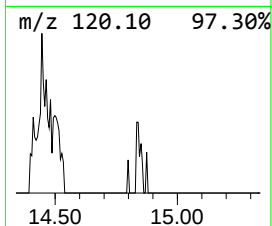
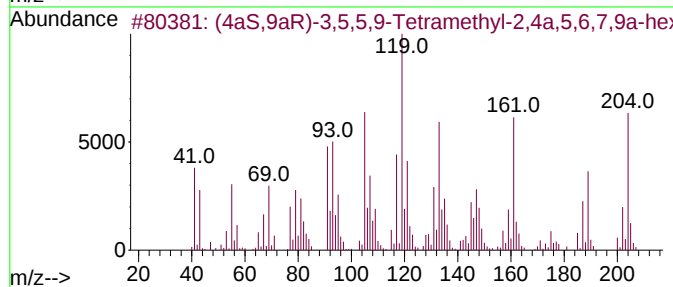
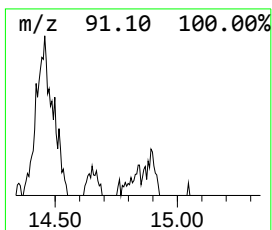
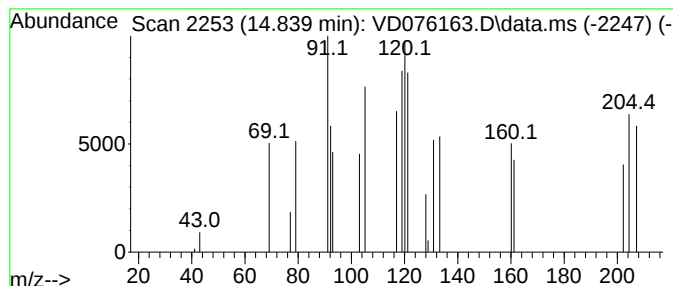
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Quant Title : SW846 8260

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

Peak Number 8 unknown14.839 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	10.03 ug/l	18986	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(4aS,9aR)-3,5,5,9-Tetramethyl-2,...	204	C15H24	053111-25-4	38		
2	Di-epi-.alpha.-cedrene-(I)	204	C15H24	021996-77-0	35		
3	Himachala-2,4-diene	204	C15H24	060909-27-5	22		
4	(5R,10S)-6,10-Dimethyl-2-(prop-1...	202	C15H22	051196-11-3	22		
5	Di-epi-.alpha.-cedrene	204	C15H24	050894-66-1	17		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD051923\
Data File : VD076163.D
Acq On : 19 May 2023 18:39
Operator : KP/SY
Sample : 02849-11
Misc : 4.92G/5.00ml/MSVOA_D/SOIL
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
TP8

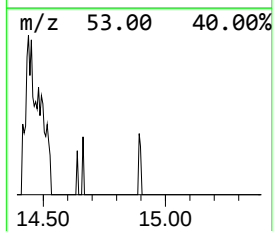
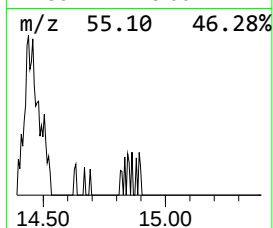
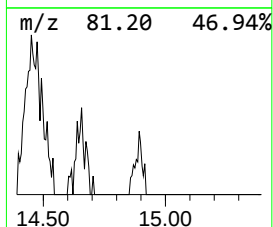
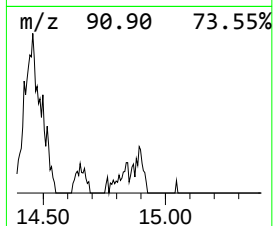
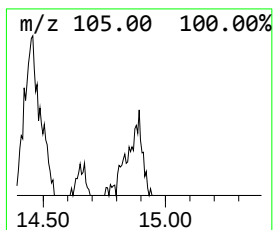
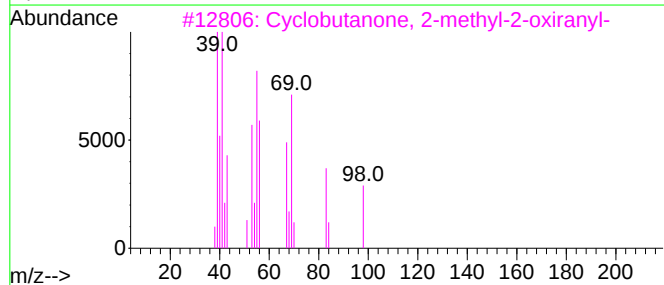
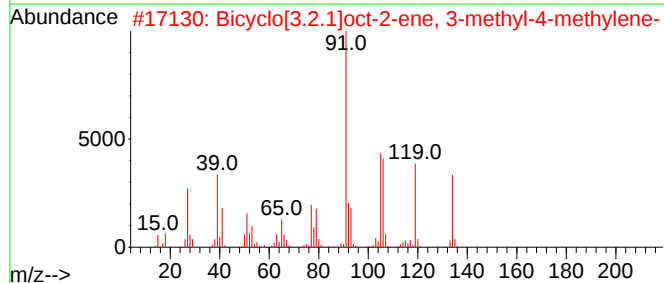
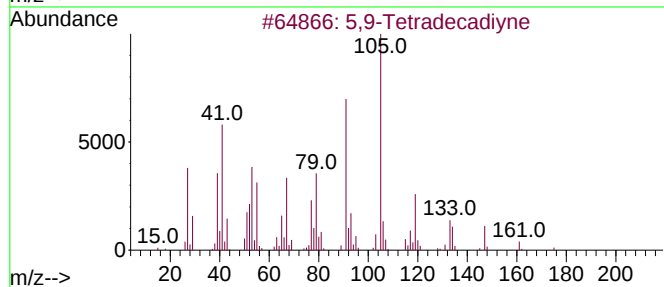
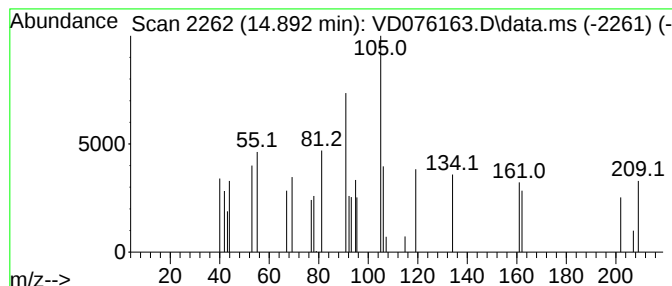
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D051523S.M
Quant Title : SW846 8260

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

Peak Number 9 unknown14.892 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.892	7.17 ug/l	13574	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,9-Tetradecadiyne	190	C14H22	051255-61-9	25		
2	Bicyclo[3.2.1]oct-2-ene, 3-methy...	134	C10H14	049826-53-1	18		
3	Cyclobutanone, 2-methyl-2-oxiranyl-	126	C7H10O2	075314-19-1	12		
4	Tetracyclo[3.3.1.1(1,8).0(2,4)]d...	134	C10H14	1000185-58-7	11		
5	3a,6-Methano-3aH-indene, 2,3,4,5...	134	C10H14	098640-10-9	10		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD051923\
Data File : VD076163.D
Acq On : 19 May 2023 18:39
Operator : KP/SY
Sample : 02849-11
Misc : 4.92G/5.00ml/MSVOA_D/SOIL
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
TP8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D051523S.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
Caryophyllene	12.398	1921.4	ug/l	1350410	3	11.581	35142	50.0
Cubenene	13.904	35.3	ug/l	66897	4	13.516	94677	50.0
cis-Muurola-4(1...	14.022	29.4	ug/l	55581	4	13.516	94677	50.0
Naphthalene, 1,...	14.457	137.7	ug/l	260647	4	13.516	94677	50.0
unknown14.657	14.657	10.5	ug/l	19799	4	13.516	94677	50.0
trans-Calamenene	14.775	9.5	ug/l	17963	4	13.516	94677	50.0
unknown14.839	14.839	10.0	ug/l	18986	4	13.516	94677	50.0
unknown14.892	14.892	7.2	ug/l	13574	4	13.516	94677	50.0