

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD102423\
 Data File : VD077402.D
 Acq On : 24 Oct 2023 18:37
 Operator : JC/SY
 Sample : 05005-04
 Misc : 5.16G/5.0ml/MSVOA_D/SOIL
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 N-3(0-5)

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\82D101723S.M

Title : SW846 8260

Signal : TIC: VD077402.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	12.216	1802	1807	1811	rVB	1050164	1488030	1.05%	0.353%
2	12.328	1822	1826	1836	rVB2	1606896	3180038	2.24%	0.755%
3	12.422	1836	1842	1847	rBV	4696723	7436081	5.25%	1.766%
4	12.763	1887	1900	1906	rBV2	28560478	46896528	33.08%	11.136%
5	12.828	1906	1911	1914	rVV	5583792	8708071	6.14%	2.068%
6	12.863	1914	1917	1919	rVV	2556188	3920229	2.77%	0.931%
7	12.898	1919	1923	1930	rVV2	9270896	16378697	11.55%	3.889%
8	13.063	1938	1951	1958	rBV	6975687	12430754	8.77%	2.952%
9	13.134	1958	1963	1970	rVB	1927493	3098610	2.19%	0.736%
10	13.216	1970	1977	1982	rBV	9581205	14778969	10.43%	3.509%
11	13.339	1990	1998	2004	rBV3	4861319	12059416	8.51%	2.864%
12	13.410	2004	2010	2015	rBV4	1256539	2300615	1.62%	0.546%
13	13.551	2026	2034	2042	rBV3	70781003	141747268	100.00%	33.660%
14	13.686	2050	2057	2059	rBV	17453777	26058910	18.38%	6.188%
15	13.722	2059	2063	2068	rVV	39282078	58381873	41.19%	13.863%
16	13.763	2068	2070	2073	rVV	2427015	2481043	1.75%	0.589%
17	13.845	2079	2084	2089	rBV2	2936753	4370076	3.08%	1.038%
18	13.916	2089	2096	2102	rVB	11667734	17651767	12.45%	4.192%
19	14.063	2115	2121	2127	rVV	17784672	26013108	18.35%	6.177%
20	14.169	2134	2139	2146	rVB3	2368910	4246099	3.00%	1.008%
21	14.304	2155	2162	2167	rBV	1310130	2063903	1.46%	0.490%
22	14.386	2167	2176	2186	rVB2	942274	1768137	1.25%	0.420%
23	14.763	2234	2240	2248	rBV2	1151672	1981123	1.40%	0.470%
24	15.333	2330	2337	2348	rVB	992883	1680946	1.19%	0.399%

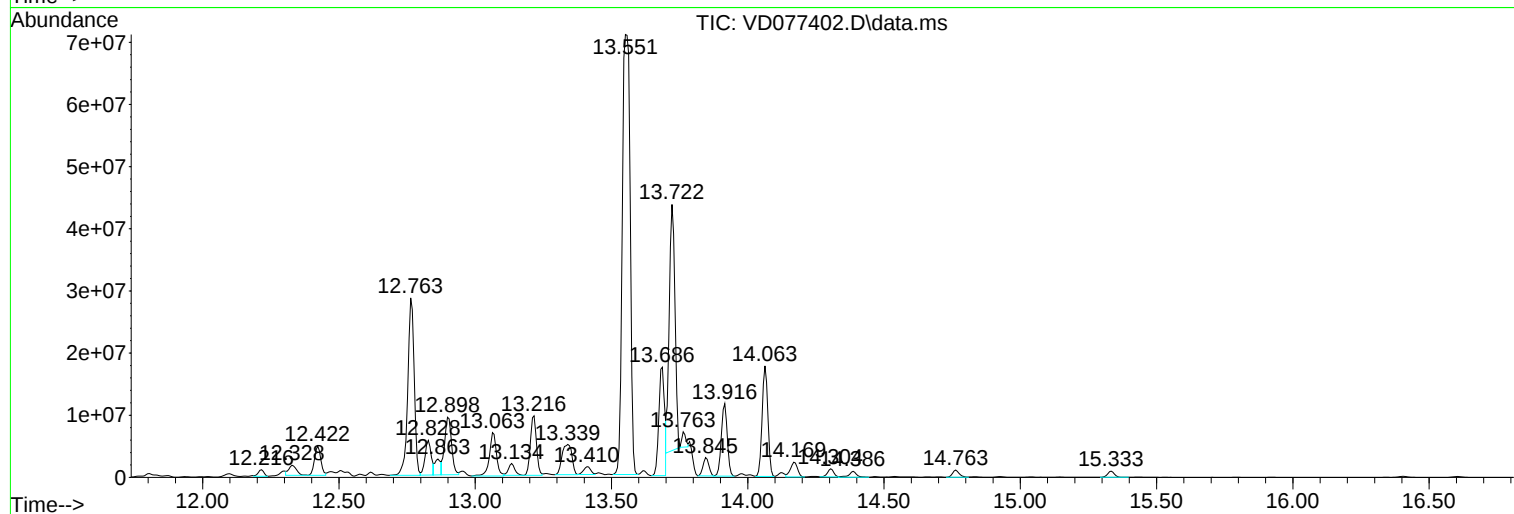
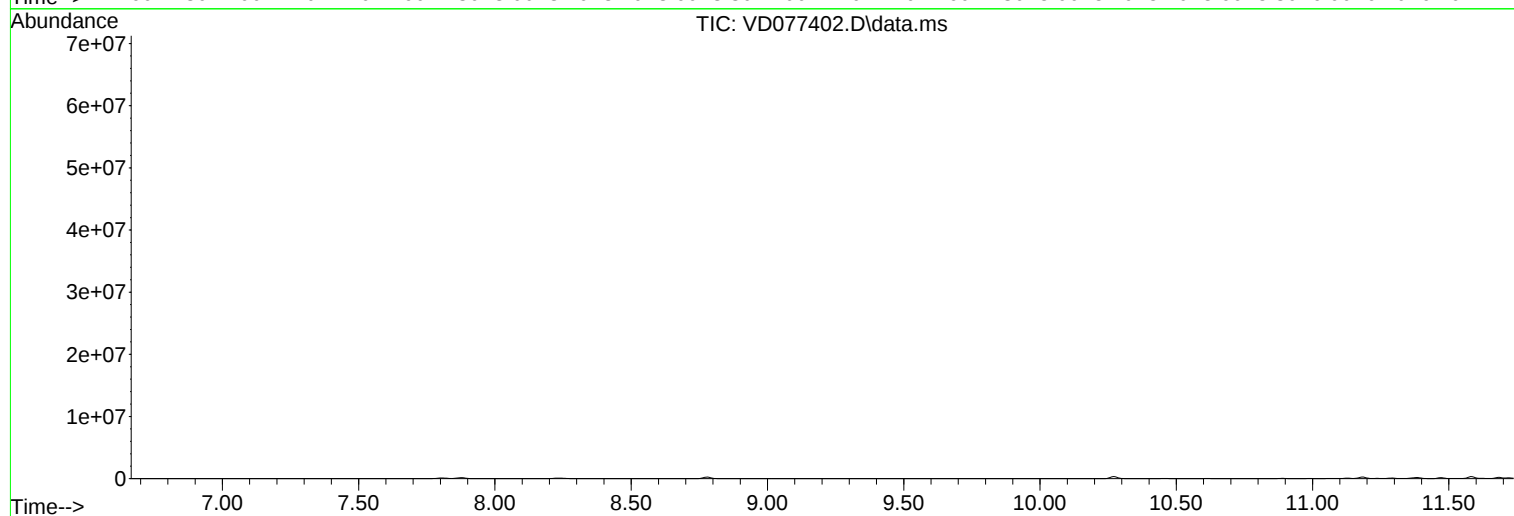
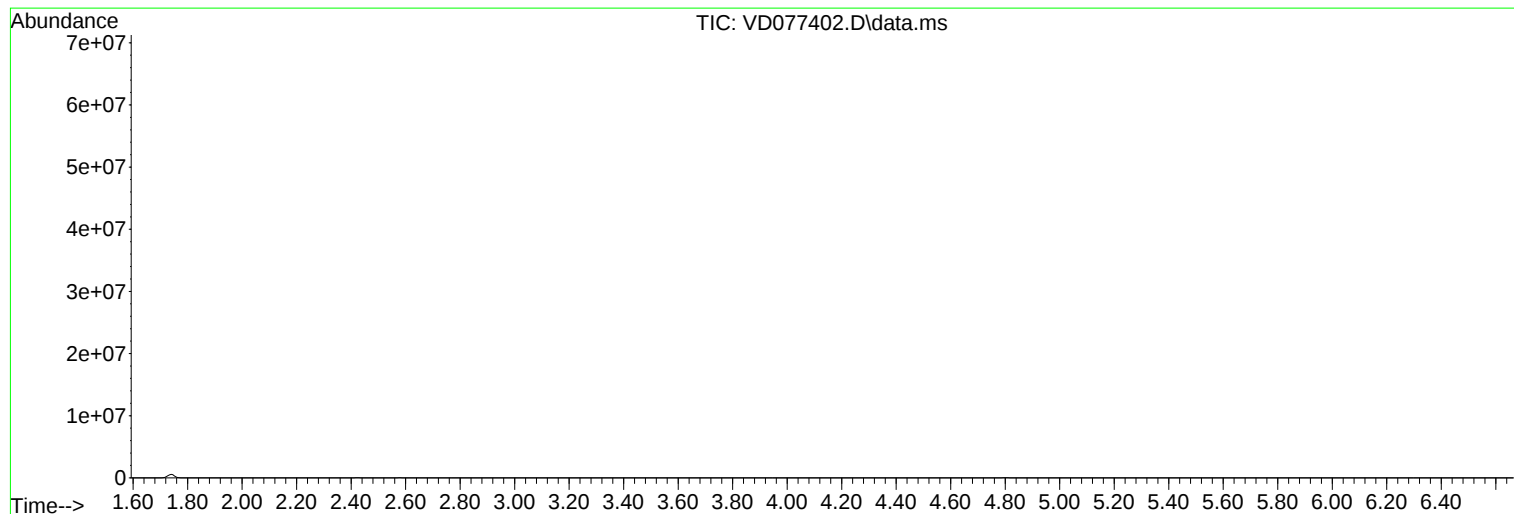
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
N-3(0-5)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101723S.M
Quant Title : SW846 8260

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



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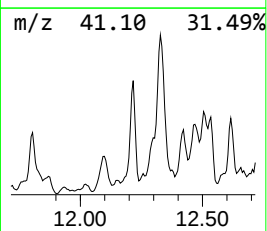
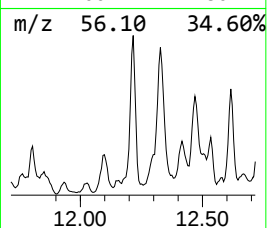
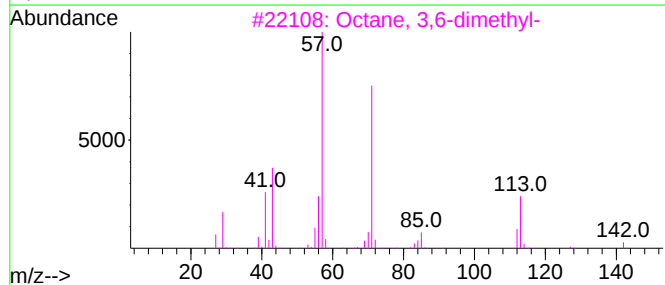
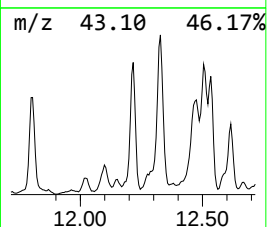
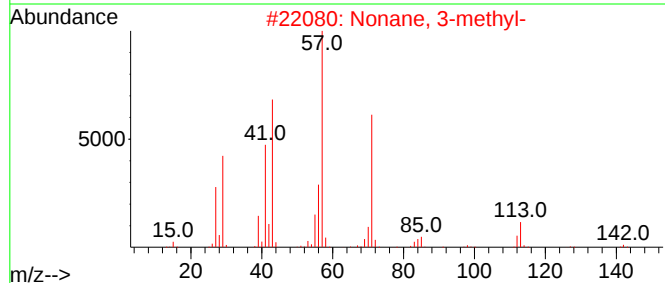
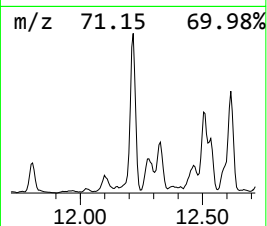
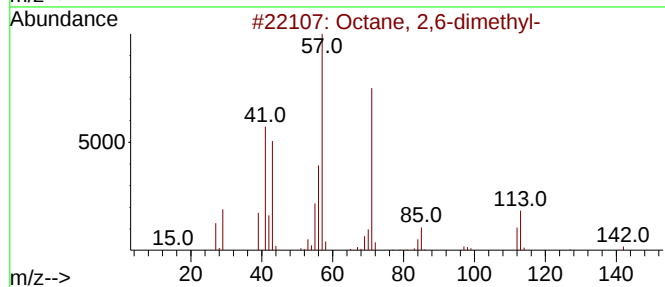
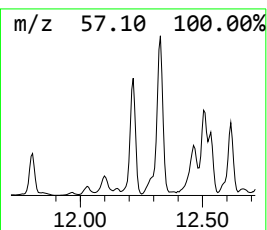
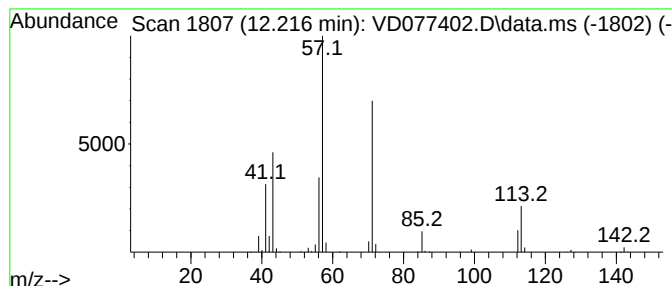
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101723S.M
Quant Title : SW846 8260

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

Peak Number 1 Octane, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.216	50.00 ug/l	1488030	Chlorobenzene-d5	11.581

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	91
2			Nonane, 3-methyl-	142	C10H22	005911-04-6	91
3			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	91
4			Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	64
5			Octane, 2,3,7-trimethyl-	156	C11H24	062016-34-6	59



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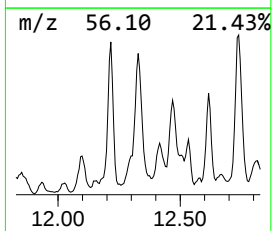
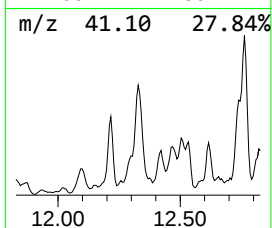
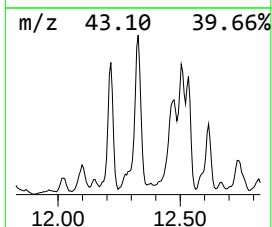
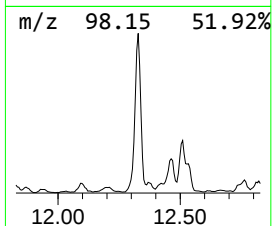
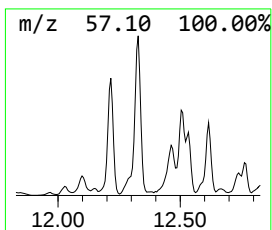
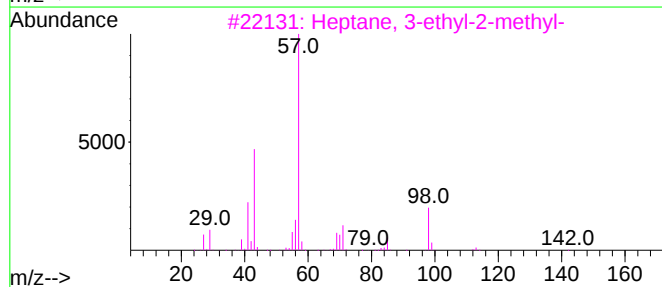
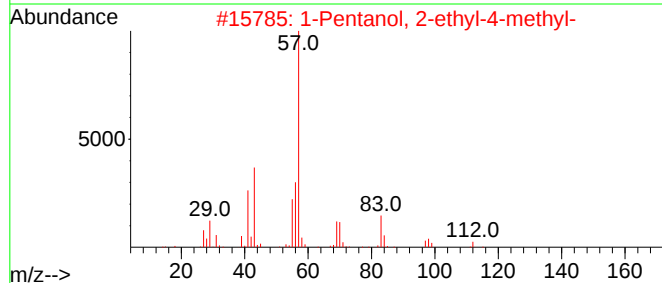
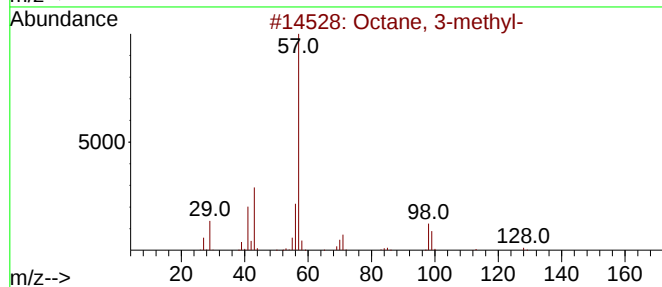
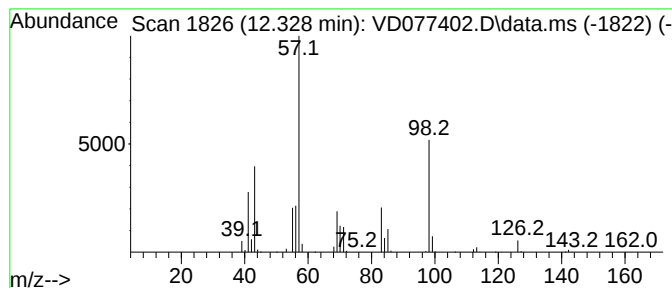
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101723S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown12.328 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.328	106.85 ug/l	3180040	Chlorobenzene-d5	11.581

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 3-methyl-	128	C9H20	002216-33-3	42
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	38
3			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	38
4			Octane, 2,5,6-trimethyl-	156	C11H24	062016-14-2	38
5			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	37



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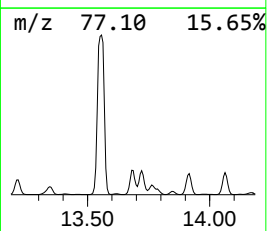
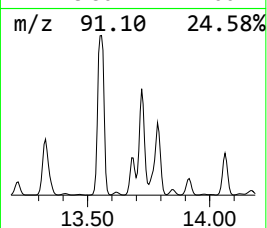
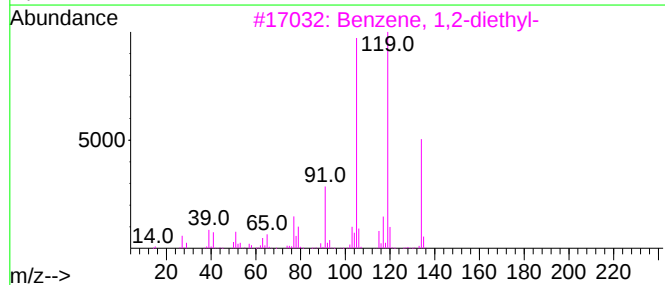
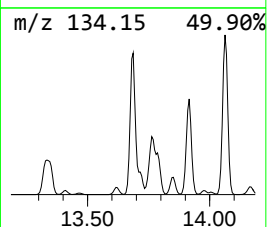
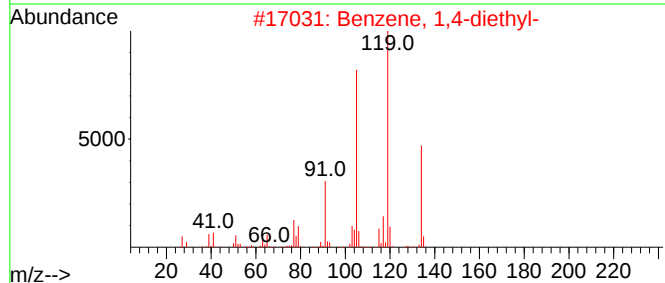
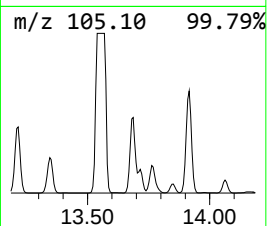
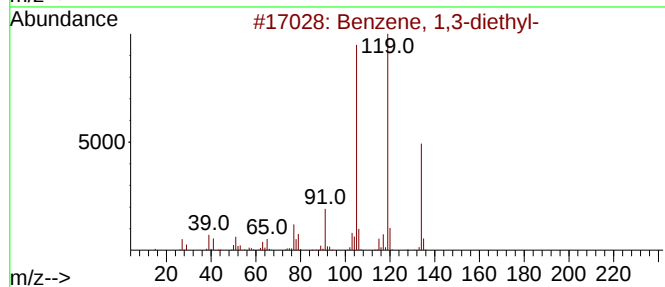
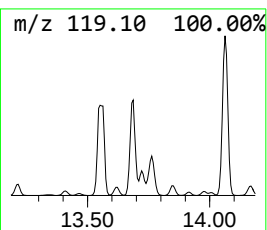
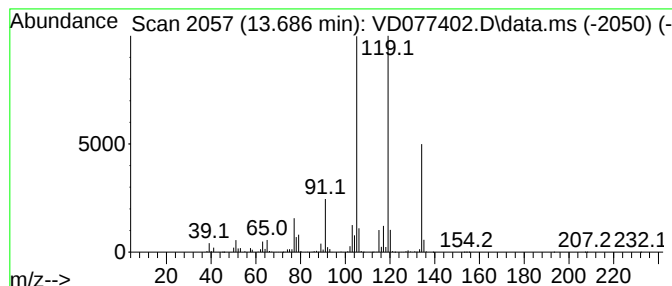
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101723S.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1,3-diethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.687	9.19 ug/l	26058900	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	97
2			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	96
3			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91
5			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	90



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Misc : 5.16G/5.0ml/MSVOA_D/SOIL
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
N-3(0-5)

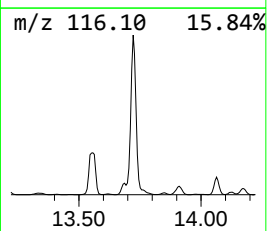
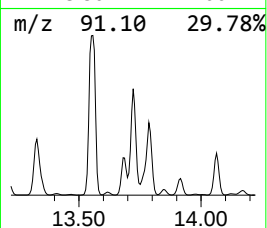
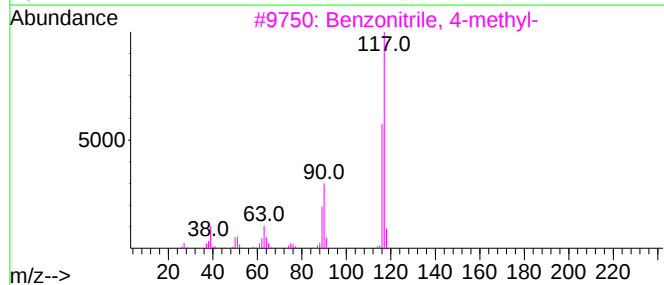
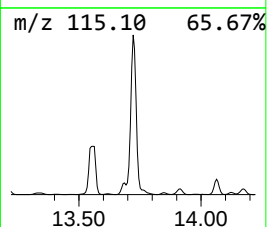
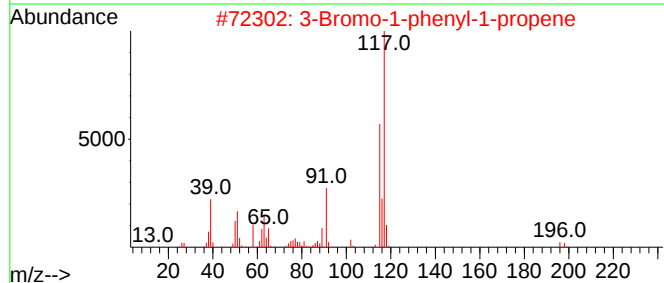
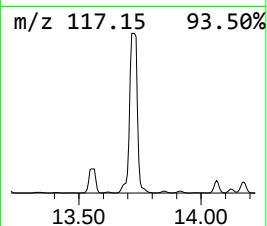
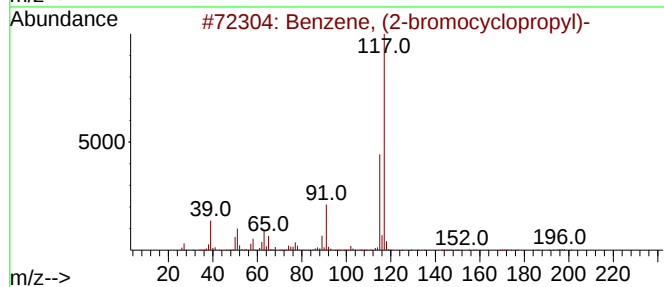
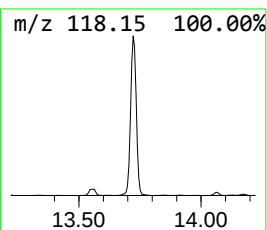
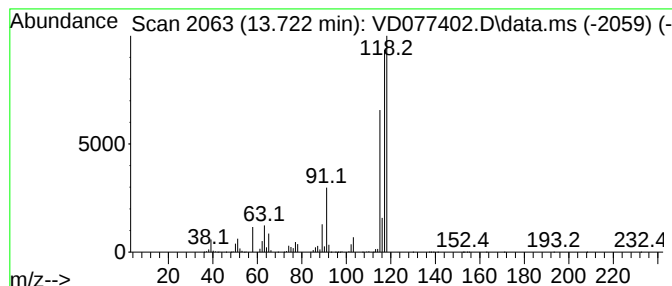
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101723S.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, (2-bromocyclopropyl)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.722	20.59 ug/l	58381900	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	50
2			3-Bromo-1-phenyl-1-propene	196	C9H9Br	004392-24-9	40
3			Benzonitrile, 4-methyl-	117	C8H7N	000104-85-8	38
4			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	37
5			Bicyclo[4.2.1]nona-2,4,7-triene,...	274	C15H14Se	072065-43-1	37



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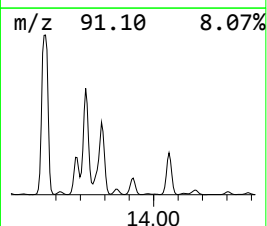
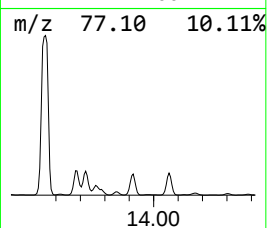
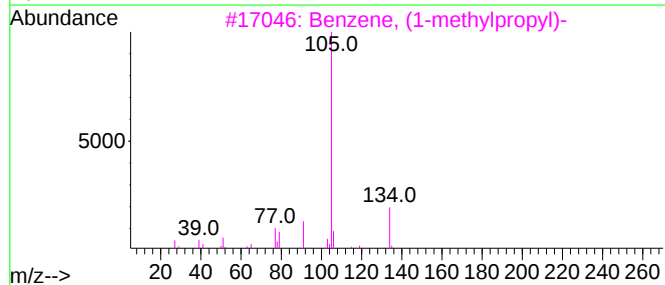
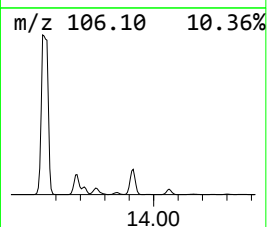
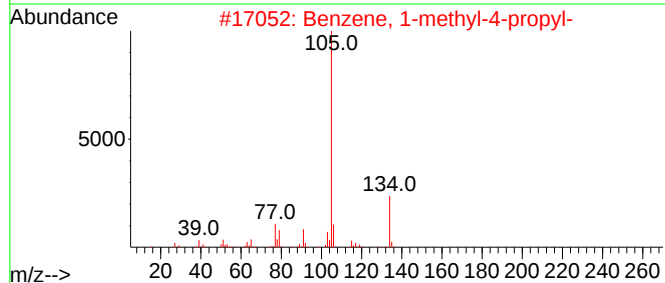
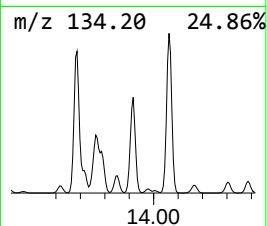
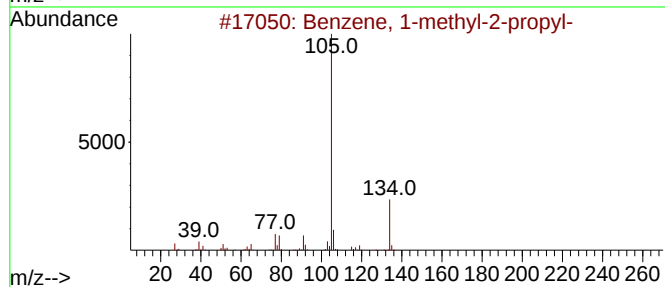
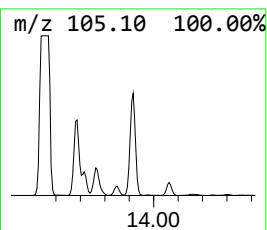
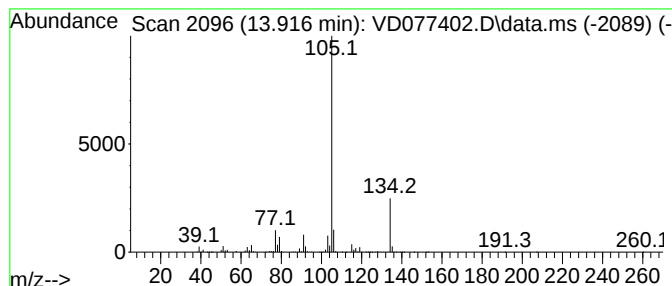
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101723S.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-methyl-2-propyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	6.23 ug/l	17651800	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	94
2			Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	94
3			Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	87
4			Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	83
5			Benzeneacetaldehyde, .alpha.-met...	134	C9H10O	000093-53-8	72



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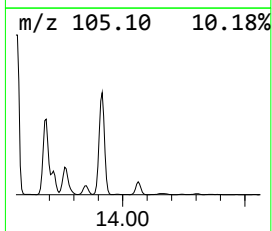
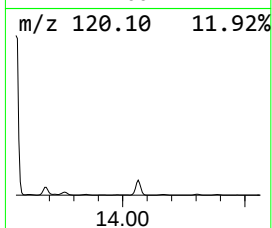
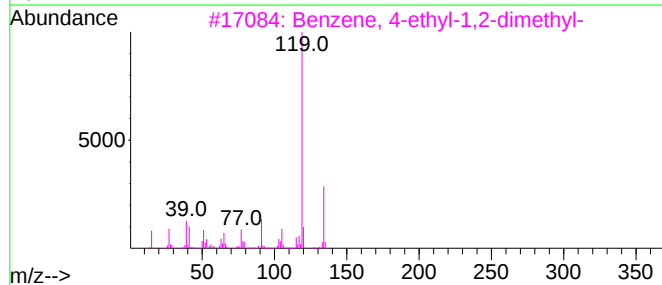
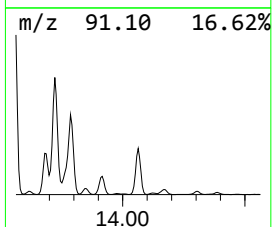
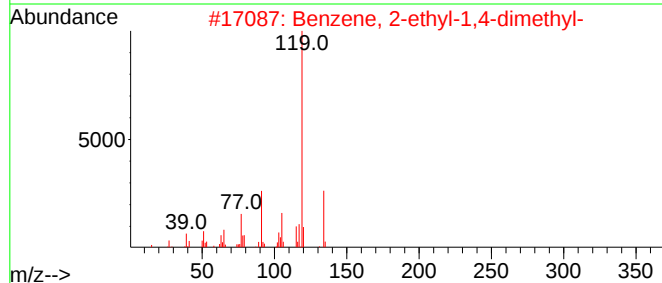
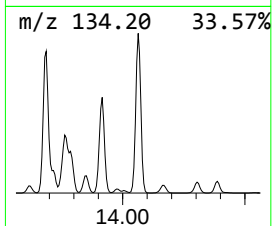
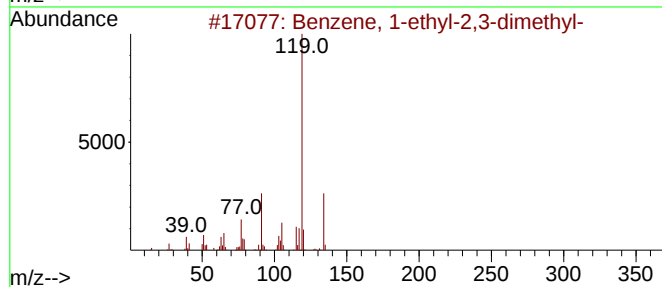
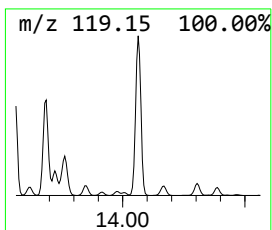
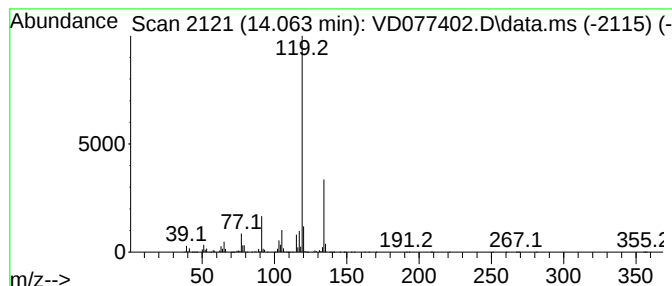
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101723S.M
Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethyl-2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.063	9.18 ug/l	26013100	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
2			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
3			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
4			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
5			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD102423\
Data File : VD077402.D
Acq On : 24 Oct 2023 18:37
Operator : JC/SY
Sample : 05005-04
Misc : 5.16G/5.0ml/MSVOA_D/SOIL
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
N-3(0-5)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101723S.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
Octane, 2,6-dim...	12.216	50.0	ug/l	1488030	3	11.581	1488030	50.0
unknown12.328	12.328	106.8	ug/l	3180040	3	11.581	1488030	50.0
Benzene, 1,3-di...	13.687	9.2	ug/l	26058900	4	13.516	141747000	50.0
Benzene, (2-bro...	13.722	20.6	ug/l	58381900	4	13.516	141747000	50.0
Benzene, 1-meth...	13.916	6.2	ug/l	17651800	4	13.516	141747000	50.0
Benzene, 1-ethy...	14.063	9.2	ug/l	26013100	4	13.516	141747000	50.0