

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD100621\
 Data File : VD070597.D
 Acq On : 06 Oct 2021 16:57
 Operator : VA/SY
 Sample : M4081-02
 Misc : 4.76G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 356

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\82D100521S.M
 Title : SW846 8260

Signal : TIC: VD070597.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.961	508	517	523	rBV6	11022	35797	1.25%	0.184%
2	7.908	1008	1018	1024	rBV	328999	808219	28.16%	4.150%
3	7.979	1024	1030	1039	rVV	505310	1163405	40.54%	5.973%
4	8.061	1039	1044	1054	rVB6	11953	32192	1.12%	0.165%
5	8.185	1057	1065	1073	rBV3	36162	79206	2.76%	0.407%
6	8.326	1080	1089	1100	rBV	308377	696301	24.26%	3.575%
7	8.450	1104	1110	1118	rVV4	15720	39985	1.39%	0.205%
8	8.538	1118	1125	1129	rVV5	13897	32894	1.15%	0.169%
9	8.602	1129	1136	1143	rVV6	20729	47753	1.66%	0.245%
10	8.714	1147	1155	1164	rVB4	16312	34777	1.21%	0.179%
11	8.861	1171	1180	1197	rBV	840558	1674117	58.33%	8.595%
12	9.355	1249	1264	1270	rBV2	97134	262445	9.14%	1.347%
13	9.532	1288	1294	1300	rBV4	19073	34574	1.20%	0.178%
14	9.620	1300	1309	1316	rVB4	30097	66334	2.31%	0.341%
15	9.767	1324	1334	1342	rBV2	39247	81032	2.82%	0.416%
16	9.973	1363	1369	1382	rVB3	99598	243905	8.50%	1.252%
17	10.108	1382	1392	1405	rBV2	71598	180374	6.28%	0.926%
18	10.332	1422	1430	1446	rBV	1549756	2870008	100.00%	14.735%
19	10.455	1446	1451	1454	rVV4	25769	47441	1.65%	0.244%
20	10.520	1454	1462	1469	rVB6	84119	207705	7.24%	1.066%
21	10.632	1475	1481	1483	rBV4	18205	30067	1.05%	0.154%
22	10.673	1483	1488	1496	rVB2	58723	111765	3.89%	0.574%
23	10.767	1496	1504	1510	rBV6	44680	109530	3.82%	0.562%
24	10.855	1516	1519	1524	rVB2	28856	41592	1.45%	0.214%
25	10.949	1524	1535	1540	rBV	85933	153309	5.34%	0.787%
26	11.044	1540	1551	1559	rBV6	37889	110951	3.87%	0.570%
27	11.120	1559	1564	1566	rVV3	31549	52321	1.82%	0.269%
28	11.185	1570	1575	1579	rVV2	83183	163601	5.70%	0.840%
29	11.238	1579	1584	1590	rVV2	154661	296981	10.35%	1.525%
30	11.296	1590	1594	1597	rVV5	22863	35148	1.22%	0.180%
31	11.344	1597	1602	1607	rVV4	61815	108029	3.76%	0.555%
32	11.426	1607	1616	1627	rVB5	109164	336674	11.73%	1.729%
33	11.520	1627	1632	1639	rBV2	129086	230654	8.04%	1.184%
34	11.638	1645	1652	1664	rVB	1281797	2187325	76.21%	11.230%
35	11.767	1671	1674	1678	rVV5	31710	54998	1.92%	0.282%
36	11.814	1678	1682	1688	rVV6	63386	145198	5.06%	0.745%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

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Sampling : 1

Min Area: 3 % of largest Peak

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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37	11.879	1688	1693	1697	rVV	86518	173731	6.05%	0.892%
38	11.920	1697	1700	1705	rVB3	70167	107991	3.76%	0.554%
39	11.979	1705	1710	1714	rBV6	19209	29847	1.04%	0.153%
40	12.143	1731	1738	1745	rBV4	90680	204208	7.12%	1.048%
41	12.255	1750	1757	1762	rVB	123515	206454	7.19%	1.060%
42	12.349	1762	1773	1774	rBV4	82673	177776	6.19%	0.913%
43	12.385	1775	1779	1787	rVB5	85699	200639	6.99%	1.030%
44	12.543	1797	1806	1814	rVB5	67736	205696	7.17%	1.056%
45	12.620	1814	1819	1829	rVB	1002765	1711056	59.62%	8.785%
46	12.708	1830	1834	1838	rVB7	24020	34304	1.20%	0.176%
47	12.785	1842	1847	1854	rVB4	83799	154460	5.38%	0.793%
48	12.867	1854	1861	1866	rBV7	28371	70568	2.46%	0.362%
49	12.938	1866	1873	1880	rVV7	98562	275796	9.61%	1.416%
50	12.996	1880	1883	1888	rVB4	47598	71733	2.50%	0.368%
51	13.085	1894	1898	1902	rBV5	28749	41165	1.43%	0.211%
52	13.132	1902	1906	1909	rVV5	22647	41038	1.43%	0.211%
53	13.173	1909	1913	1921	rVB3	99638	167768	5.85%	0.861%
54	13.449	1953	1960	1965	rBV5	67328	150690	5.25%	0.774%
55	13.490	1965	1967	1971	rVV4	44244	60993	2.13%	0.313%
56	13.561	1973	1979	1988	rVB	1201156	2007890	69.96%	10.309%
57	13.885	2029	2034	2038	rBV6	70299	118435	4.13%	0.608%
58	14.096	2064	2070	2075	rVB7	31618	63438	2.21%	0.326%
59	14.208	2083	2089	2095	rBV6	35538	73417	2.56%	0.377%
60	14.279	2096	2101	2106	rVB8	16735	34305	1.20%	0.176%
61	14.390	2115	2120	2125	rVV5	42840	68276	2.38%	0.351%
62	14.555	2144	2148	2153	rVB7	26004	40872	1.42%	0.210%
63	14.802	2187	2190	2196	rBV7	26444	59053	2.06%	0.303%
64	14.861	2196	2200	2207	rVB7	23428	48124	1.68%	0.247%
65	15.079	2232	2237	2242	rVB8	17877	32565	1.13%	0.167%
66	16.402	2457	2462	2471	rBV10	14616	38172	1.33%	0.196%

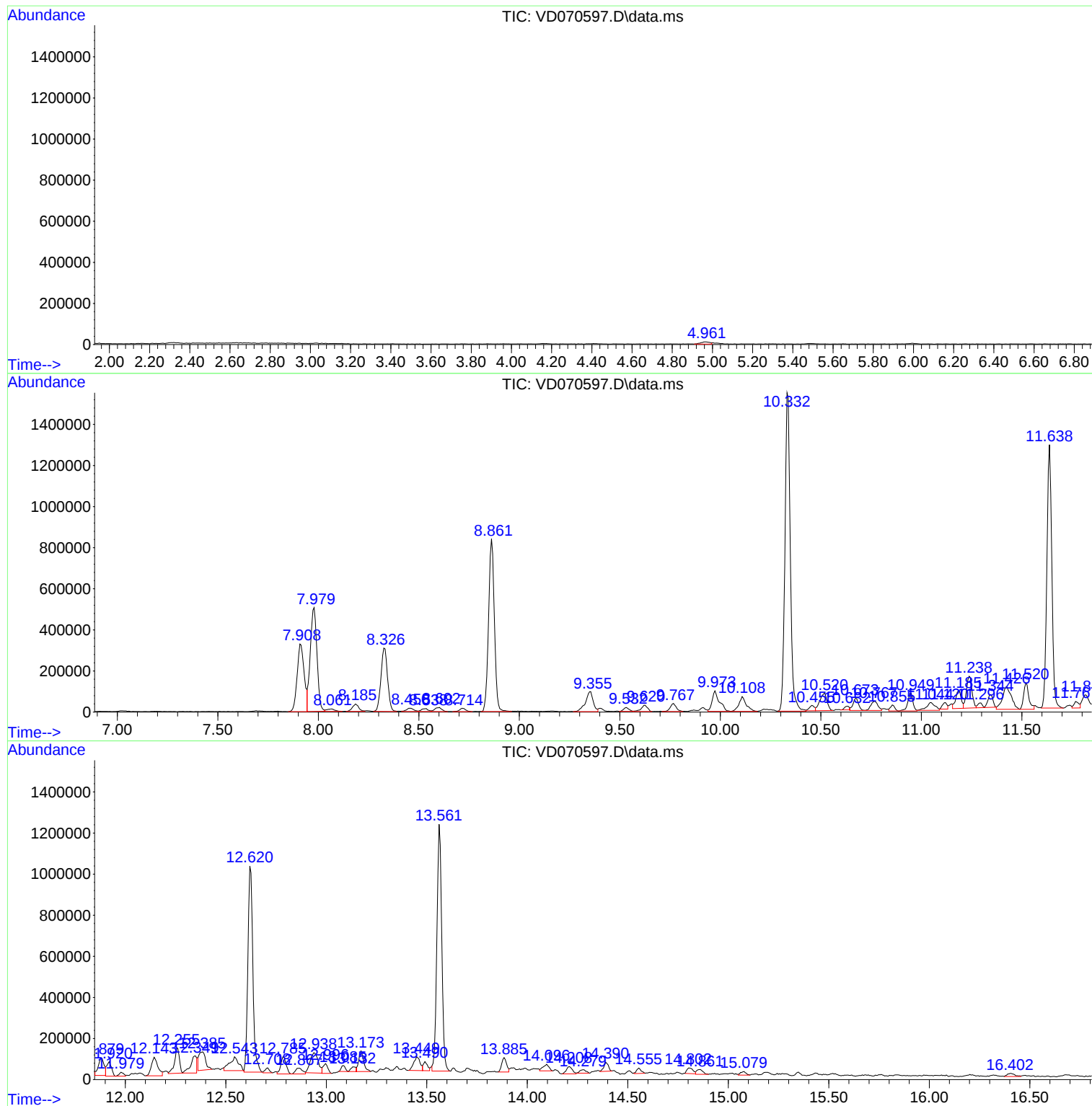
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D100521S.M
Quant Title : SW846 8260

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



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Misc : 4.76G/5.00ml/MSVOA_D/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
356

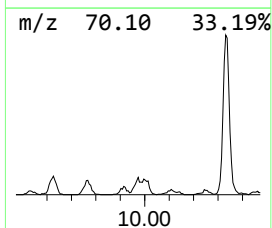
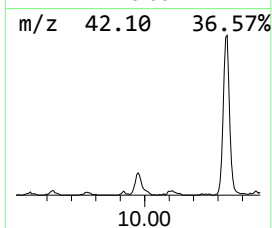
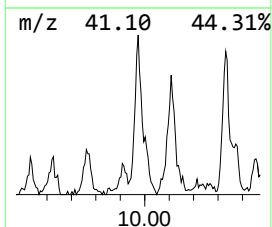
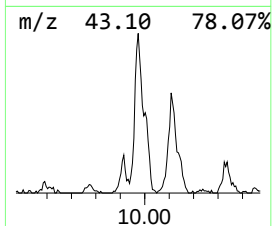
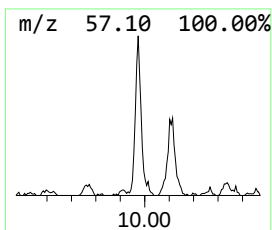
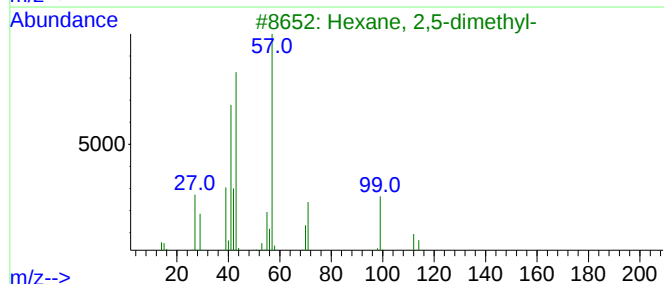
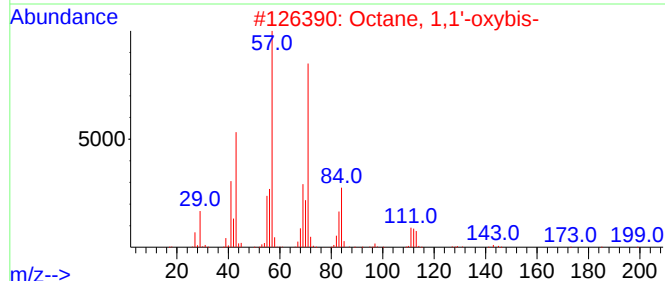
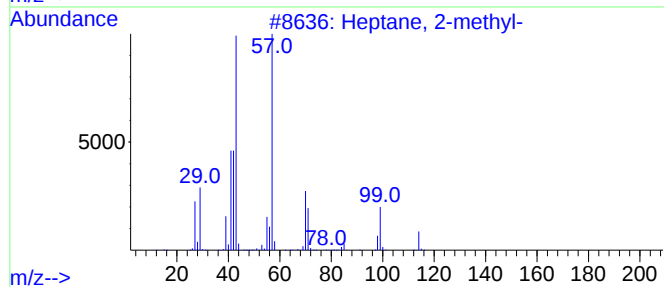
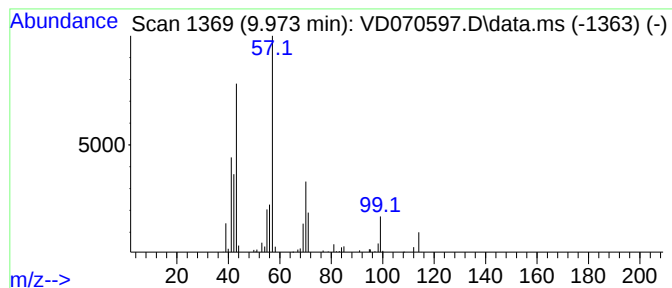
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D100521S.M
Quant Title : SW846 8260

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

Peak Number 1 Heptane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.973	7.28 ug/l	243905	1,4-Difluorobenzene	8.861

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2-methyl-	114	C8H18	000592-27-8	81
2			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	47
3			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	43
4			Heptane, 4-propyl-	142	C10H22	003178-29-8	38
5			Decane, 2,5,6-trimethyl-	184	C13H28	062108-23-0	38



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Instrument :
MSVOA_D
ClientSampled :
356

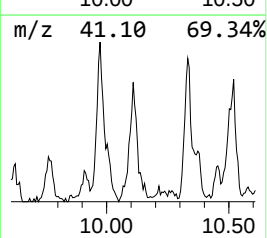
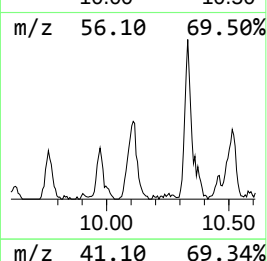
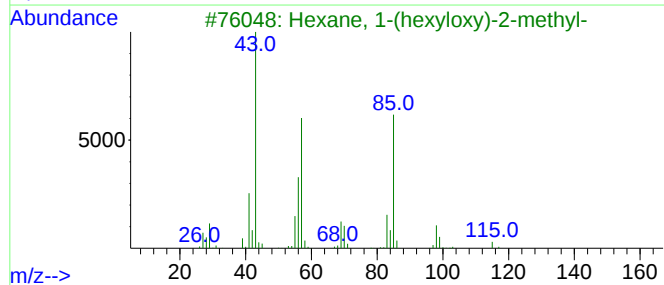
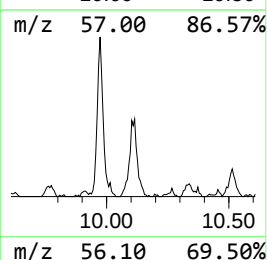
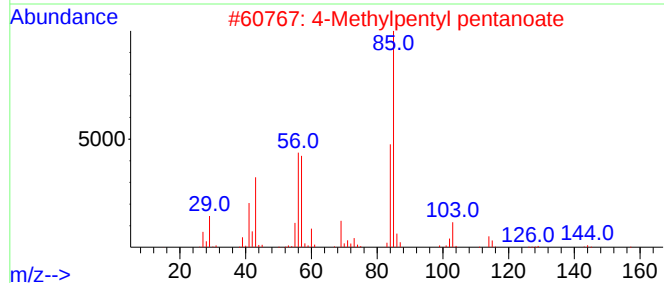
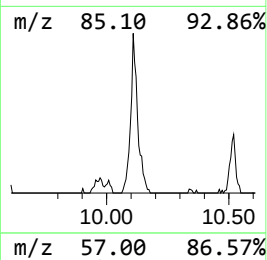
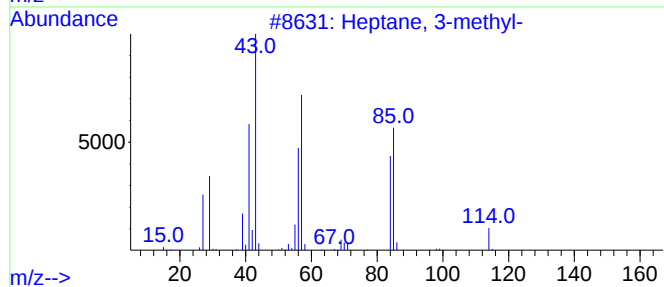
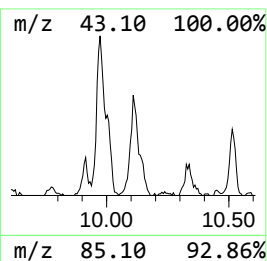
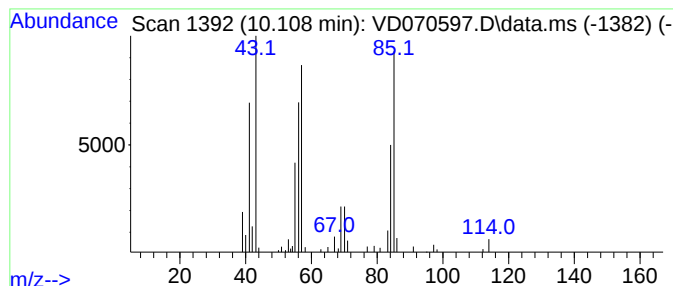
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D100521S.M
Quant Title : SW846 8260

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

Peak Number 2 Heptane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.108	5.39 ug/l	180374	1,4-Difluorobenzene	8.861

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-methyl-	114	C8H18	000589-81-1	83
2			4-Methylpentyl pentanoate	186	C11H22O2	035852-47-2	59
3			Hexane, 1-(hexyloxy)-2-methyl-	200	C13H28O	074421-17-3	59
4			Hexane, 2-methyl-	100	C7H16	000591-76-4	53
5			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	53



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Misc : 4.76G/5.00ml/MSVOA_D/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
356

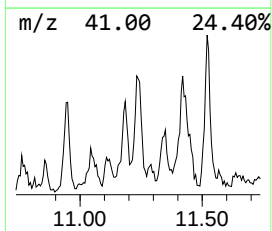
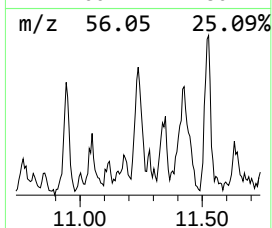
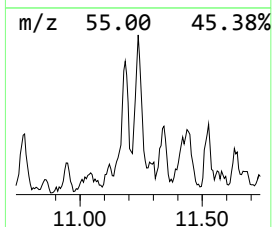
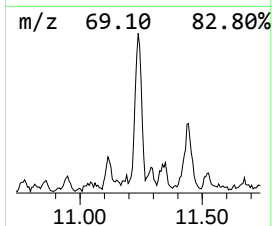
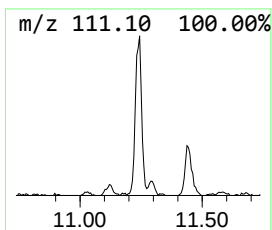
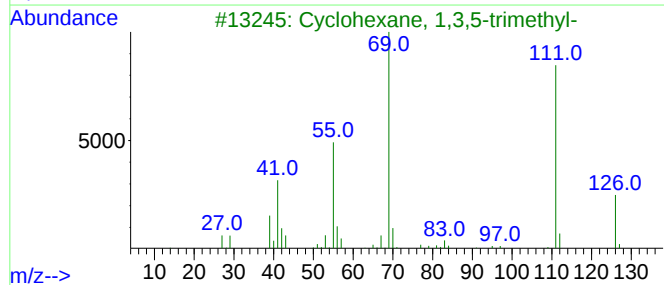
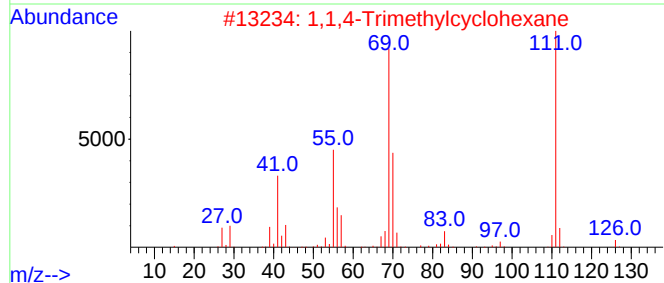
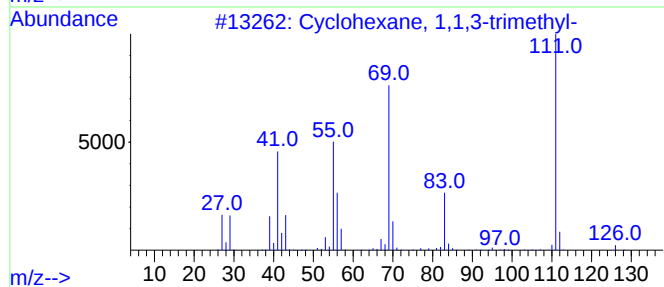
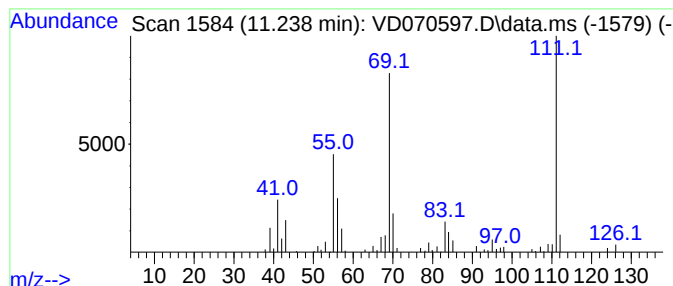
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D100521S.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.238	6.79 ug/l	296981	Chlorobenzene-d5	11.638

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	90
2			1,1,4-Trimethylcyclohexane	126	C9H18	007094-27-1	80
3			Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	64
4			Cyclohexane, 1,3,5-trimethyl-, (...)	126	C9H18	001795-27-3	64
5			Cyclooctane, butyl-	168	C12H24	016538-93-5	50



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Instrument :
MSVOA_D
ClientSampled :
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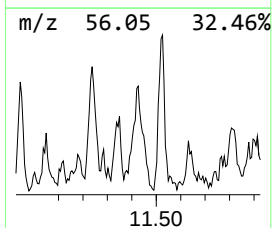
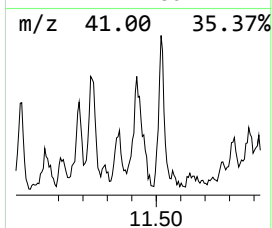
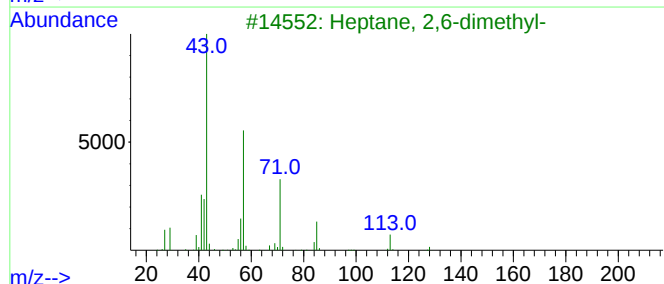
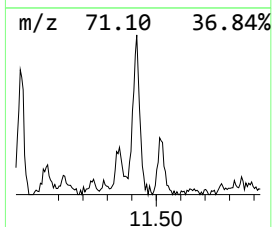
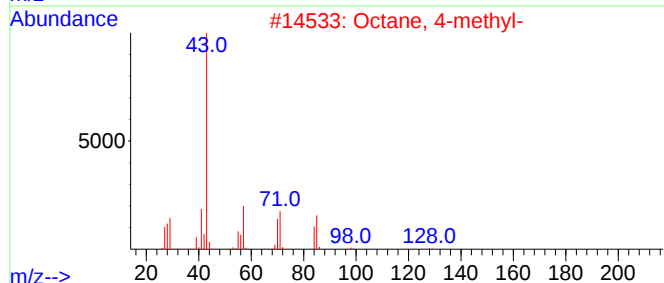
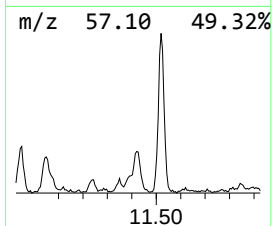
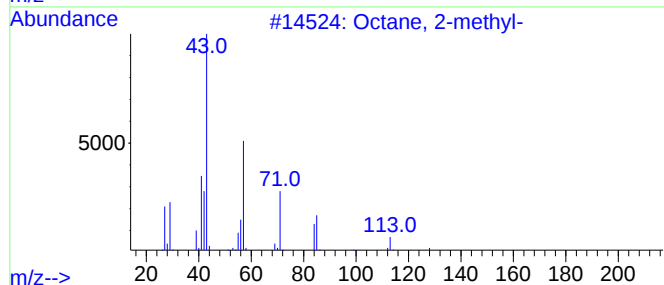
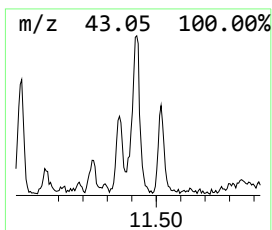
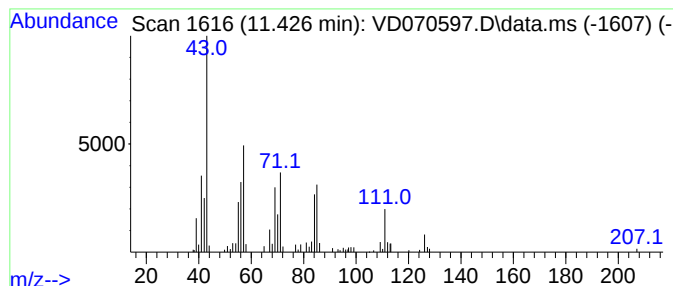
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D100521S.M
Quant Title : SW846 8260

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

Peak Number 4 unknown11.426 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.426	7.70 ug/l	336674	Chlorobenzene-d5	11.638

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-methyl-		128	C9H20	003221-61-2	46	
2	Octane, 4-methyl-		128	C9H20	002216-34-4	43	
3	Heptane, 2,6-dimethyl-		128	C9H20	001072-05-5	38	
4	Hexane, 2,3,4-trimethyl-		128	C9H20	000921-47-1	38	
5	Octane		114	C8H18	000111-65-9	38	



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Sample : M4081-02
Misc : 4.76G/5.00ml/MSVOA_D/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
356

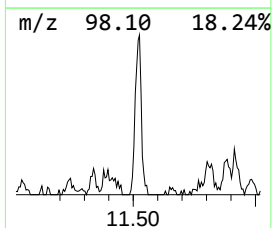
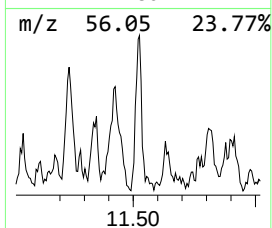
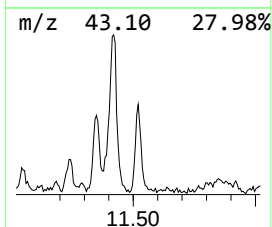
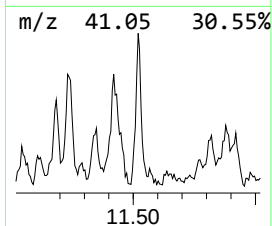
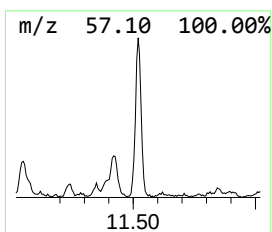
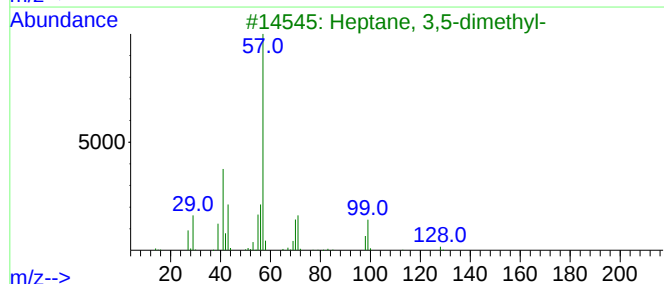
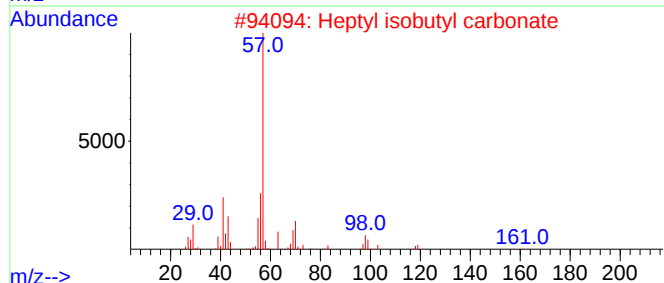
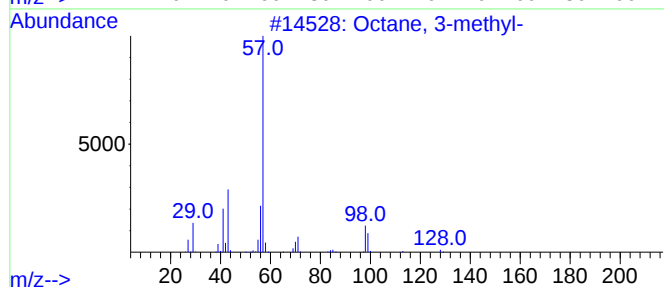
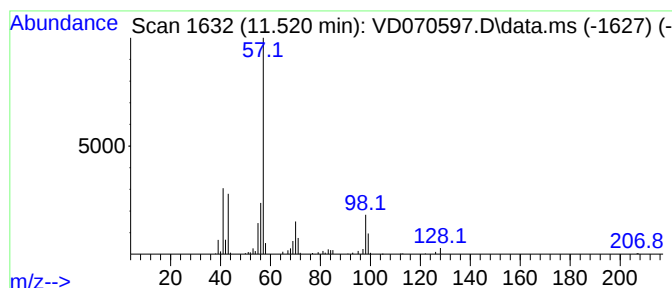
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Quant Title : SW846 8260

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

Peak Number 5 Octane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.520	5.27 ug/l	230654	Chlorobenzene-d5	11.638

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 3-methyl-	128	C9H20	002216-33-3	80
2			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	59
3			Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	58
4			Carbonic acid, butyl heptyl ester	216	C12H24O3	1000314-63-4	53
5			Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD100621\
Data File : VD070597.D
Acq On : 06 Oct 2021 16:57
Operator : VA/SY
Sample : M4081-02
Misc : 4.76G/5.00ml/MSVOA_D/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
356

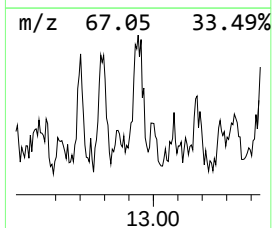
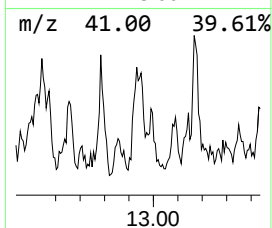
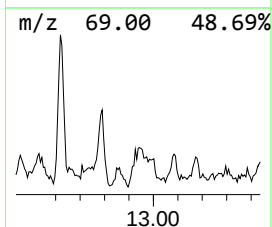
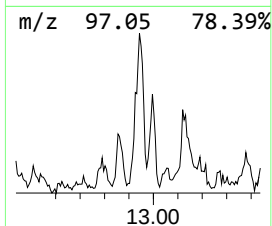
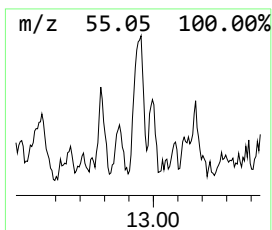
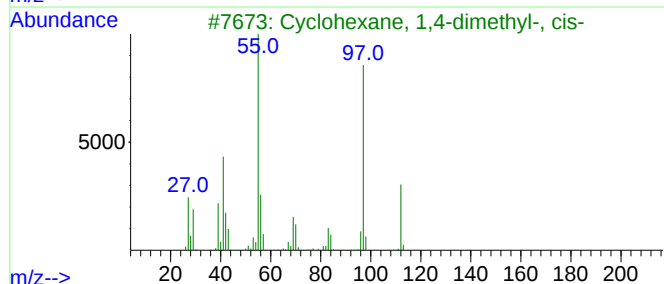
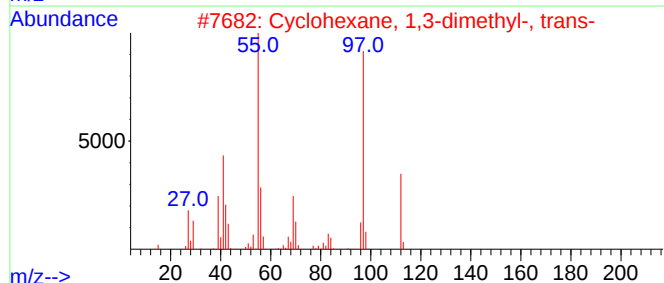
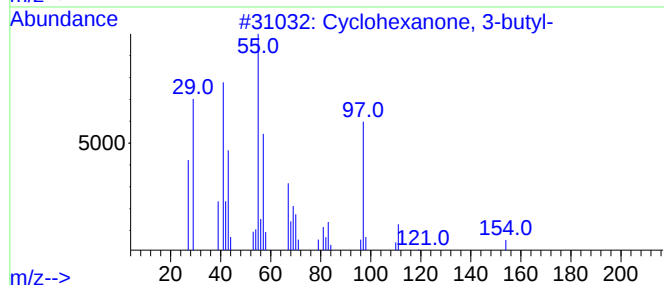
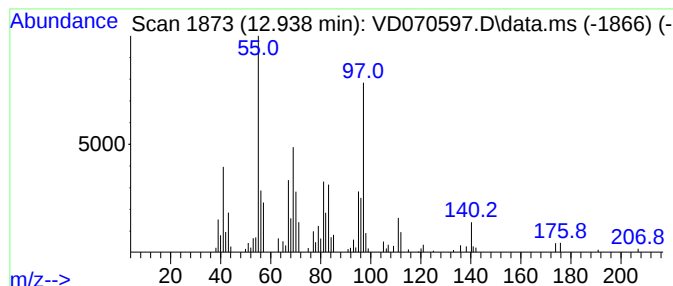
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Quant Title : SW846 8260

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

Peak Number 6 Cyclohexanone, 3-butyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.938	6.87 ug/l	275796	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 3-butyl-	154	C10H18O	039178-69-3	50
2			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	49
3			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	49
4			m-Menthane, (1S,3R)-(+)-	140	C10H20	013837-66-6	47
5			Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD100621\
Data File : VD070597.D
Acq On : 06 Oct 2021 16:57
Operator : VA/SY
Sample : M4081-02
Misc : 4.76G/5.00ml/MSVOA_D/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
356

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D100521S.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
Heptane, 2-methyl-	9.973	7.3	ug/l	243905	2	8.861	1674120	50.0
Heptane, 3-methyl-	10.108	5.4	ug/l	180374	2	8.861	1674120	50.0
Cyclohexane, 1,...	11.238	6.8	ug/l	296981	3	11.638	2187330	50.0
unknown11.426	11.426	7.7	ug/l	336674	3	11.638	2187330	50.0
Octane, 3-methyl-	11.520	5.3	ug/l	230654	3	11.638	2187330	50.0
Cyclohexanone, ...	12.938	6.9	ug/l	275796	4	13.561	2007890	50.0