

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112224\
 Data File : VY020412.D
 Acq On : 22 Nov 2024 14:50
 Operator : SY/MD
 Sample : P4946-02
 Misc : 5.09g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 BW-2

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\82Y111924S.M

Title : SW846 8260

Signal : TIC: VY020412.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.116	384	393	403	rBV2	2302	7193	1.16%	0.316%
2	6.896	840	849	857	rBV2	6822	20878	3.36%	0.917%
3	7.640	961	971	977	rBV	39128	92759	14.95%	4.073%
4	7.713	977	983	994	rVB	69957	158253	25.50%	6.949%
5	8.067	1030	1041	1056	rBV2	33746	78598	12.67%	3.451%
6	8.621	1123	1132	1144	rVB	106906	215188	34.68%	9.449%
7	10.005	1353	1359	1365	rBV3	3743	6753	1.09%	0.297%
8	10.109	1369	1376	1385	rBV	162310	279868	45.10%	12.289%
9	10.511	1437	1442	1449	rVB2	7520	14942	2.41%	0.656%
10	10.871	1495	1501	1508	rBV6	4570	9154	1.48%	0.402%
11	11.420	1583	1591	1605	rBV	146251	234768	37.83%	10.309%
12	11.956	1672	1679	1685	rBV	11067	17254	2.78%	0.758%
13	12.267	1724	1730	1735	rBV2	6792	11366	1.83%	0.499%
14	12.413	1747	1754	1763	rVB2	97396	170030	27.40%	7.466%
15	12.535	1766	1774	1783	rBV5	3144	7345	1.18%	0.323%
16	12.694	1791	1800	1804	rBV	18045	31722	5.11%	1.393%
17	13.200	1875	1883	1889	rBV3	5276	8312	1.34%	0.365%
18	13.352	1901	1908	1914	rBV	109071	168000	27.07%	7.377%
19	13.456	1918	1925	1939	rBV	398141	620577	100.00%	27.251%
20	13.834	1981	1987	1993	rBV8	3851	9526	1.54%	0.418%
21	13.889	1993	1996	2002	rVB2	4293	6718	1.08%	0.295%
22	14.078	2023	2027	2031	rBV4	4046	7698	1.24%	0.338%
23	14.133	2031	2036	2041	rVB5	12589	20412	3.29%	0.896%
24	14.376	2068	2076	2088	rVB7	8924	28883	4.65%	1.268%
25	14.474	2088	2092	2098	rBV6	4663	9176	1.48%	0.403%
26	14.535	2099	2102	2107	rVB5	4588	6683	1.08%	0.293%
27	14.889	2156	2160	2168	rVB6	7534	18761	3.02%	0.824%
28	14.962	2168	2172	2185	rBV8	6458	16481	2.66%	0.724%

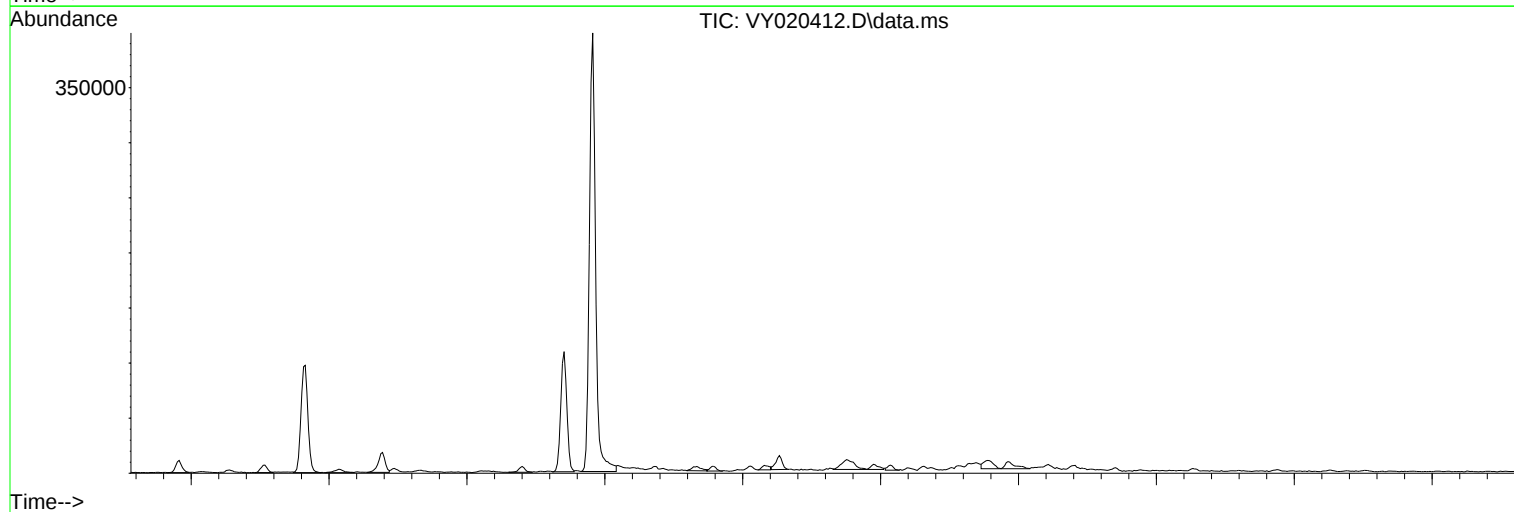
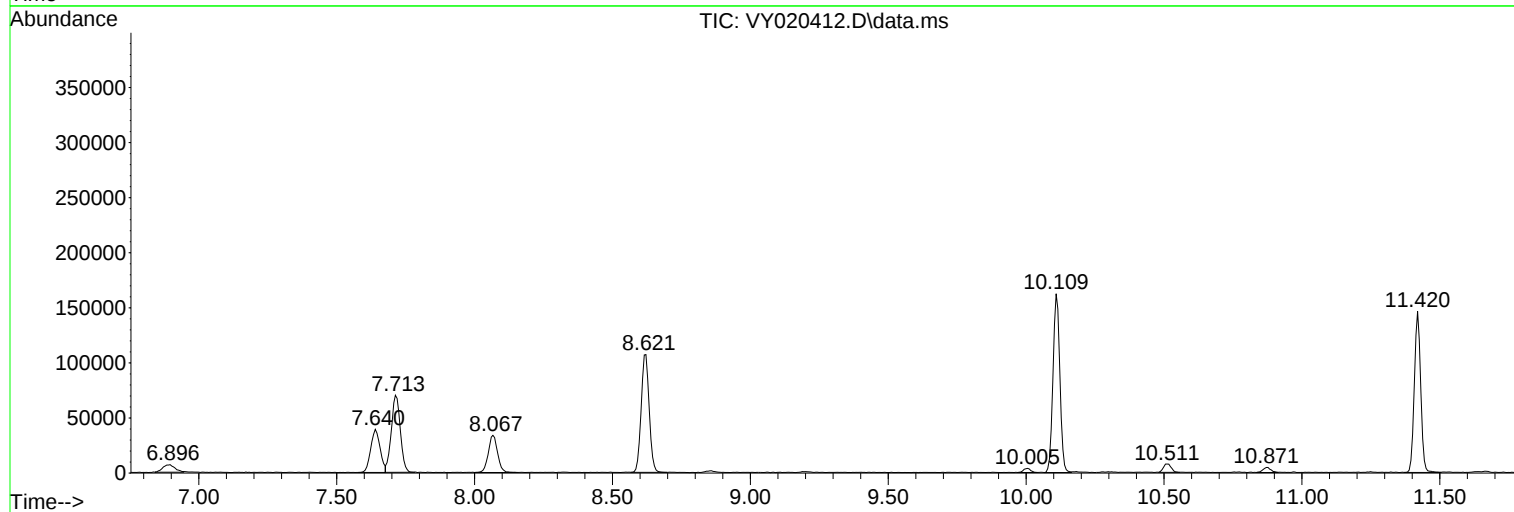
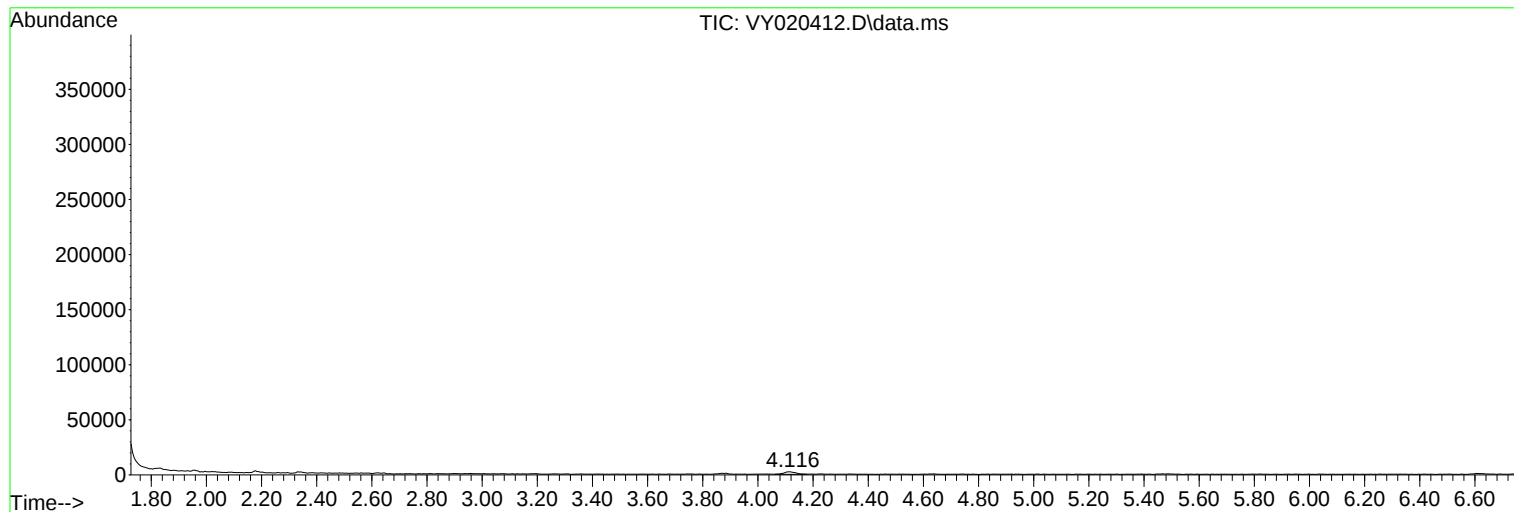
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111924S.M
Quant Title : SW846 8260

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



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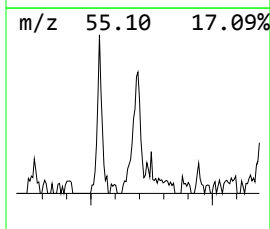
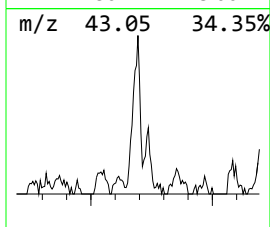
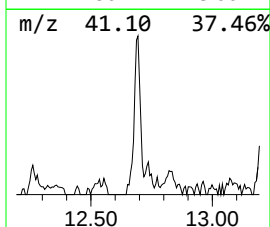
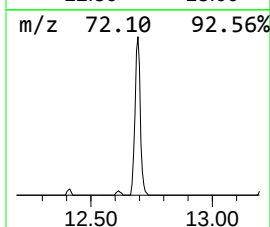
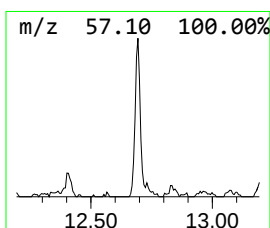
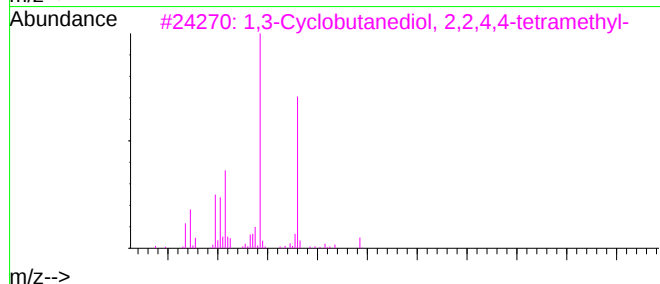
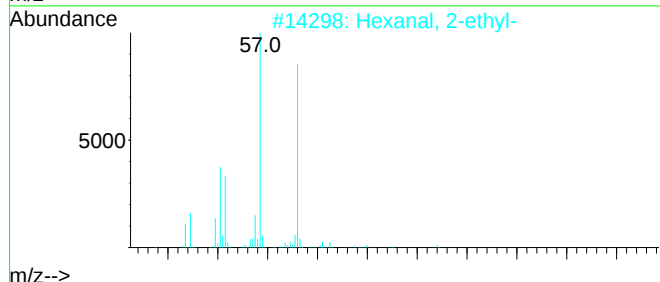
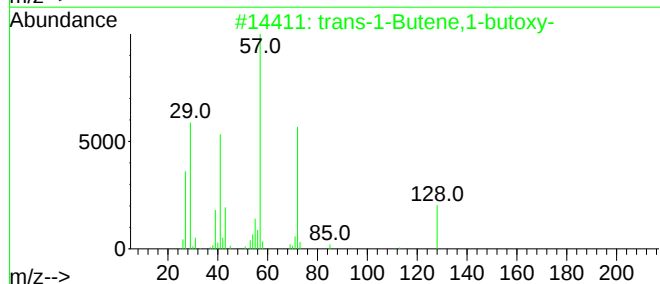
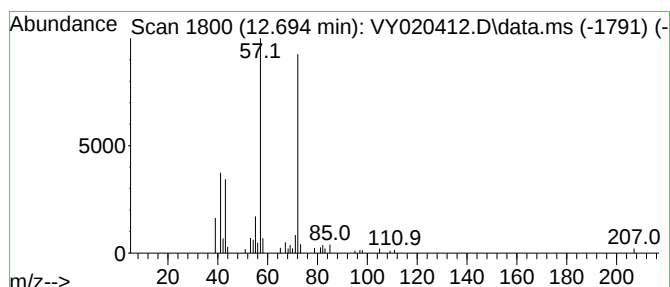
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111924S.M
Quant Title : SW846 8260

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

Peak Number 2 trans-1-Butene,1-butoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.694	9.44 ug/l	31722	1,4-Dichlorobenzene-d4	13.352

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-1-Butene,1-butoxy-	128	C8H16O	1000139-52-8	72
2	Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	72
3	1,3-Cyclobutanediol, 2,2,4,4-tet...	144	C8H16O2	003010-96-6	64
4	Pentane, 1-(1-butenyloxy)-, (E)-	142	C9H18O	054004-25-0	59
5	Methylephedrine	179	C11H17NO	000552-79-4	53



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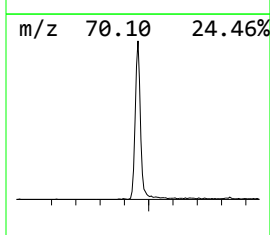
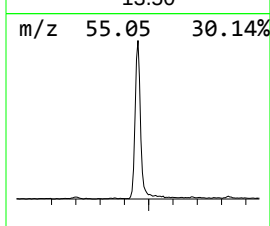
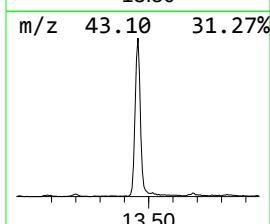
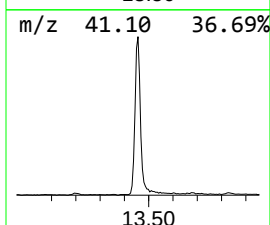
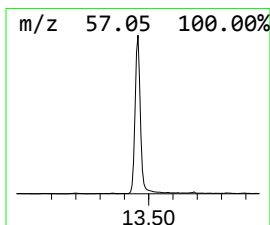
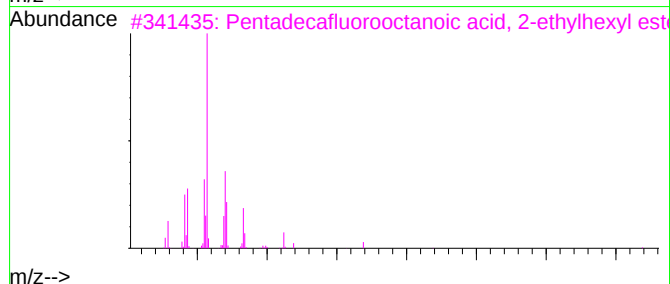
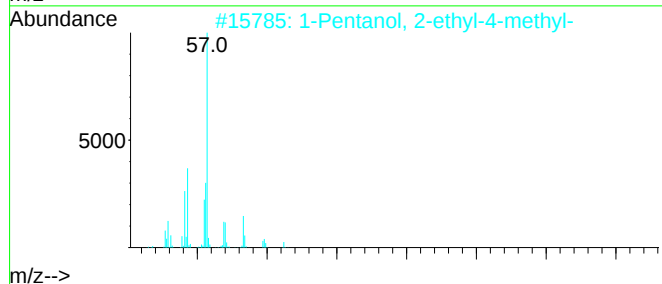
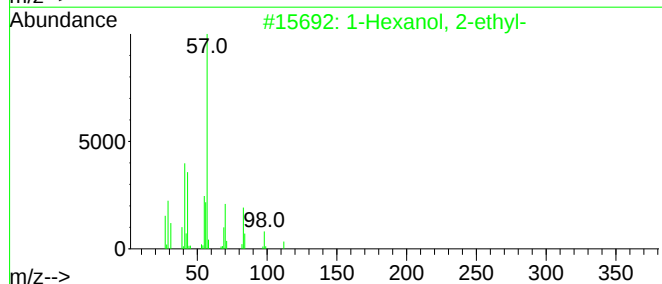
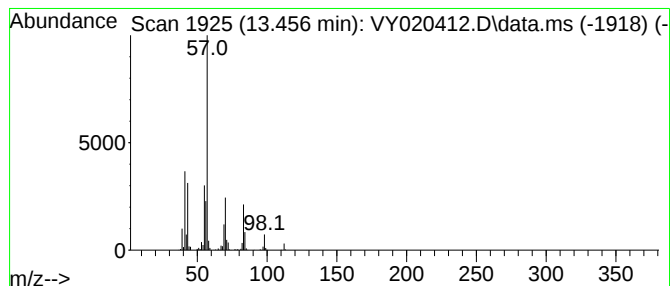
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111924S.M
Quant Title : SW846 8260

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.456	184.70 ug/l	620577	1,4-Dichlorobenzene-d4	13.352

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3	Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	53
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47



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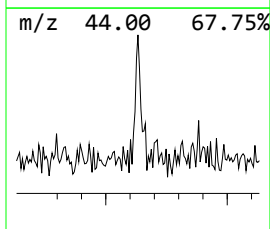
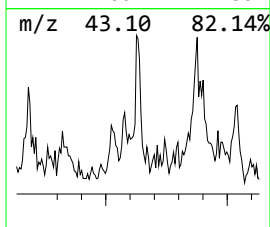
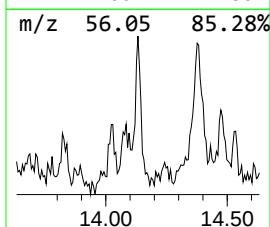
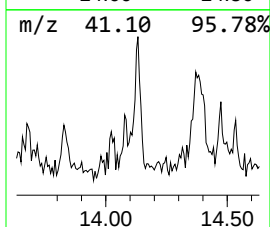
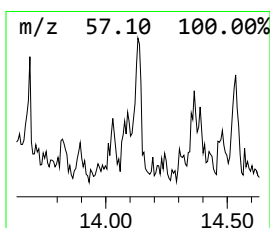
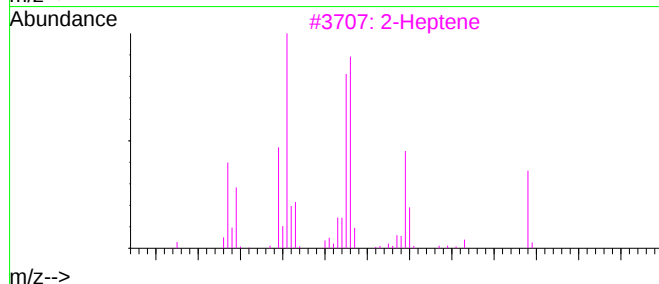
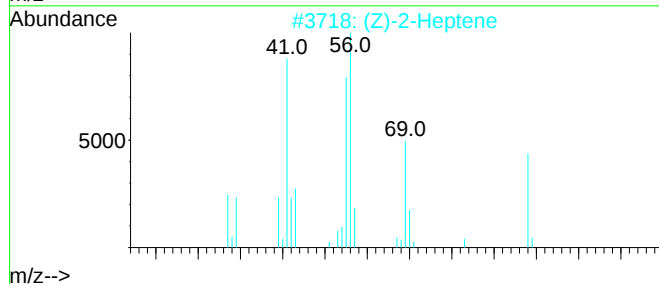
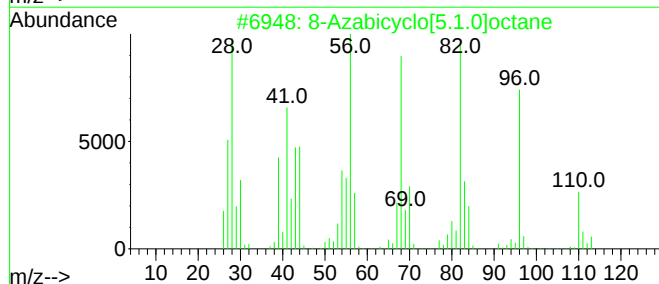
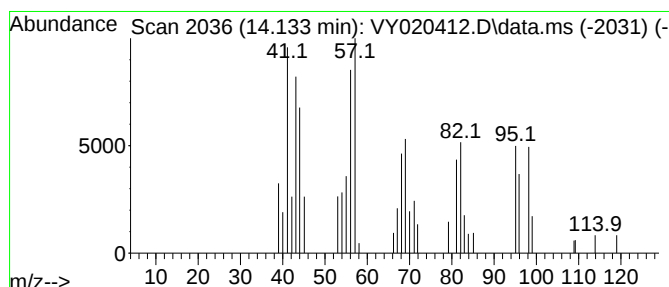
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown14.133 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.133	6.08 ug/l	20412	1,4-Dichlorobenzene-d4	13.352

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-Azabicyclo[5.1.0]octane	111	C7H13N	000286-44-2	38
2	(Z)-2-Heptene	98	C7H14	006443-92-1	27
3	2-Heptene	98	C7H14	000592-77-8	27
4	3-Buten-1-ol, 3-methyl-	86	C5H10O	000763-32-6	22
5	(1S,2S)-(+)-1,2-Diaminocyclohexane	114	C6H14N2	021436-03-3	18



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ALS Vial : 13 Sample Multiplier: 1

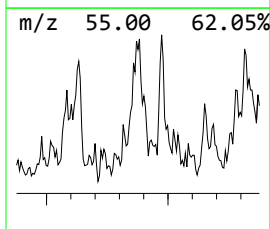
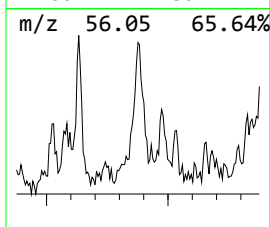
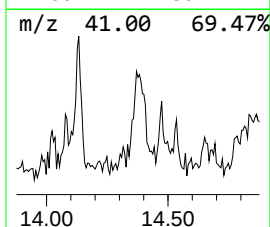
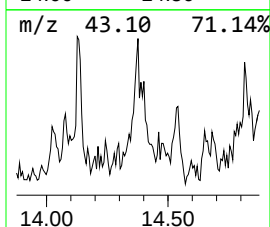
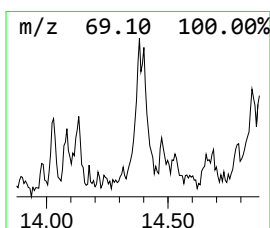
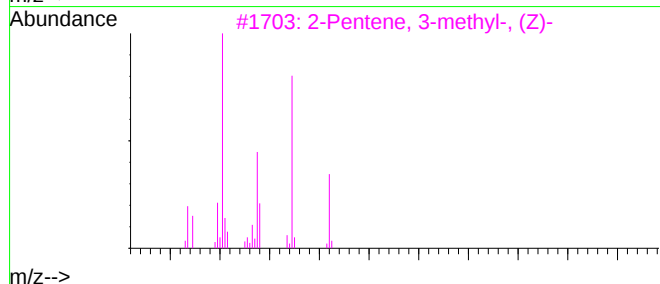
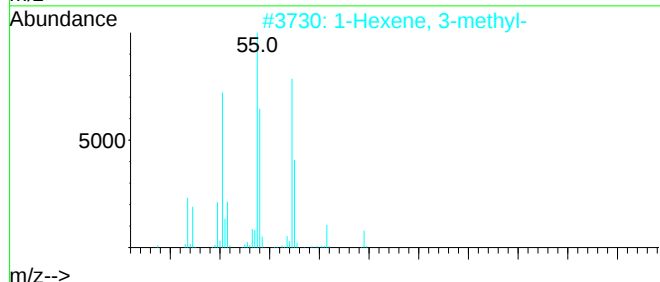
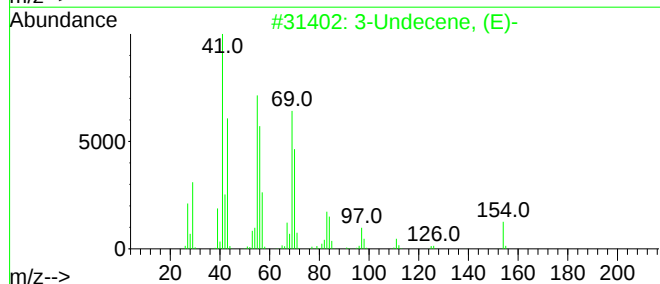
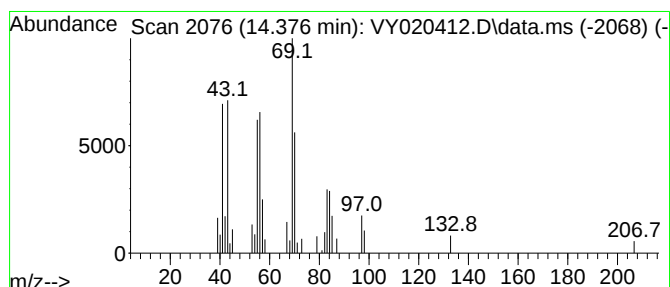
Instrument :
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 3-Undecene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.376	8.60 ug/l	28883	1,4-Dichlorobenzene-d4	13.352	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Undecene, (E)-	154	C11H22	001002-68-2	78
2	1-Hexene, 3-methyl-	98	C7H14	003404-61-3	68
3	2-Pentene, 3-methyl-, (Z)-	84	C6H12	000922-62-3	46
4	3-Methyl-2-hexene	98	C7H14	017618-77-8	46
5	Cyclopropane, 1,1-diethyl-	98	C7H14	001003-19-6	43



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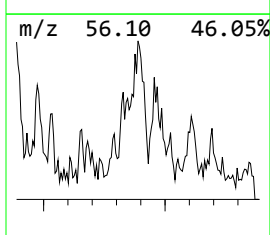
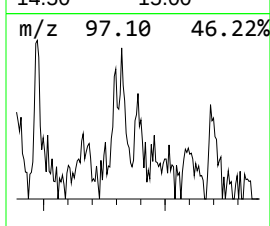
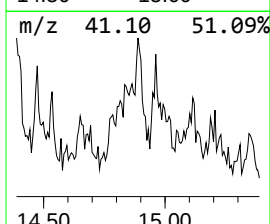
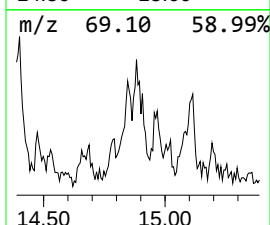
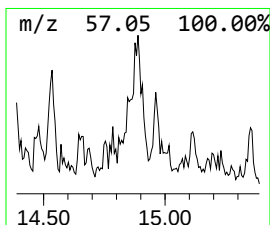
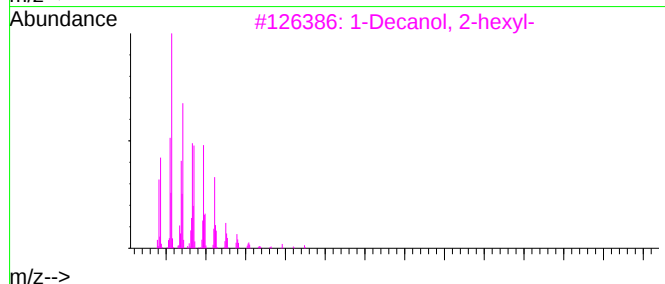
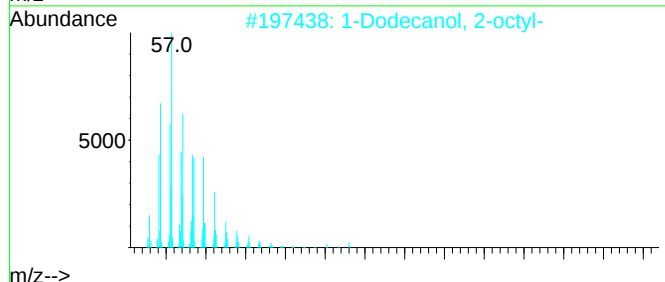
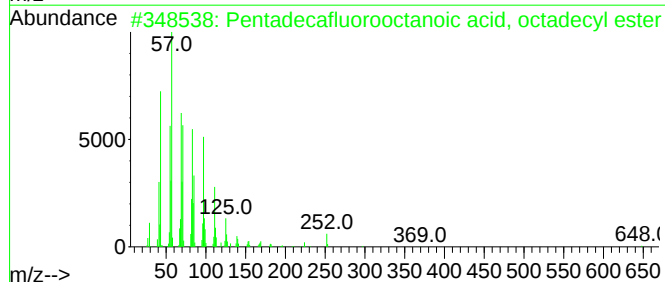
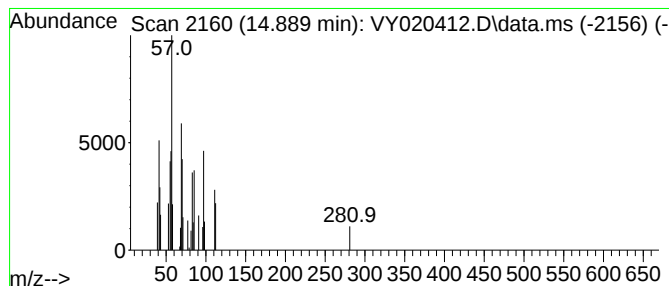
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Quant Title : SW846 8260

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

Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.889	5.58 ug/l	18761	1,4-Dichlorobenzene-d4	13.352

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	50
2	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	50
3	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	47
4	2-Undecene, 6-methyl-, (Z)-	168	C12H24	074630-43-6	47
5	2-Butenedioic acid (E)-, bis(2-e...	340	C20H36O4	000141-02-6	43



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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
trans-1-Butene,...	12.694	9.4	ug/l	31722	4	13.352	168000	50.0
1-Hexanol, 2-et...	13.456	184.7	ug/l	620577	4	13.352	168000	50.0
unknown14.133	14.133	6.1	ug/l	20412	4	13.352	168000	50.0
3-Undecene, (E)-	14.376	8.6	ug/l	28883	4	13.352	168000	50.0
Pentadecafluoro...	14.889	5.6	ug/l	18761	4	13.352	168000	50.0