

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY072123\
 Data File : VY014737.D
 Acq On : 21 Jul 2023 11:23
 Operator : SY/MD
 Sample : 03681-08
 Misc : 2.38g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 RPTP-3-GRAB-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_Y\methods\82Y071323S.M
 Title : SW846 8260

Signal : TIC: VY014737.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.046	32	37	42	rBV2	10130	23232	3.33%	0.688%
2	2.095	42	45	56	rVB	10325	22691	3.26%	0.672%
3	2.582	120	125	130	rBV2	6551	13902	2.00%	0.412%
4	3.606	291	293	296	rBV2	11246	12821	1.84%	0.380%
5	6.460	752	761	773	rBV	34762	135344	19.42%	4.009%
6	7.764	954	975	983	rBV4	51866	239747	34.41%	7.102%
7	8.130	1028	1035	1036	rBV6	9334	16135	2.32%	0.478%
8	8.685	1116	1126	1132	rBV3	45578	156098	22.40%	4.624%
9	10.178	1360	1371	1403	rBV	116301	696830	100.00%	20.643%
10	10.611	1431	1442	1456	rVV2	77616	229346	32.91%	6.794%
11	10.745	1456	1464	1474	rVB	15167	33201	4.76%	0.984%
12	10.941	1490	1496	1507	rVV3	5625	17154	2.46%	0.508%
13	11.062	1510	1516	1528	rVB4	11234	24011	3.45%	0.711%
14	11.227	1536	1543	1549	rBV6	7412	18880	2.71%	0.559%
15	11.300	1549	1555	1567	rVB3	17783	40424	5.80%	1.197%
16	11.520	1578	1591	1601	rBV2	81586	313300	44.96%	9.281%
17	11.599	1601	1604	1609	rVV5	9230	19586	2.81%	0.580%
18	11.648	1610	1612	1617	rVV2	6795	12413	1.78%	0.368%
19	11.715	1617	1623	1636	rVB5	9513	34674	4.98%	1.027%
20	12.038	1668	1676	1685	rVB10	3598	11707	1.68%	0.347%
21	12.343	1720	1726	1736	rBV3	11254	25233	3.62%	0.747%
22	12.501	1744	1752	1759	rBV	324515	596834	85.65%	17.680%
23	12.587	1762	1766	1771	rVB4	6607	12346	1.77%	0.366%
24	12.648	1771	1776	1780	rBV4	7921	15937	2.29%	0.472%
25	12.739	1786	1791	1794	rBV6	6609	12464	1.79%	0.369%
26	12.812	1796	1803	1809	rVV4	26028	57123	8.20%	1.692%
27	12.873	1810	1813	1817	rVB3	12426	17872	2.56%	0.529%
28	13.050	1837	1842	1852	rVB4	22989	51358	7.37%	1.521%
29	13.178	1858	1863	1870	rVB9	10245	25947	3.72%	0.769%
30	13.257	1871	1876	1878	rVV3	8130	15214	2.18%	0.451%
31	13.294	1878	1882	1885	rVV3	21792	38879	5.58%	1.152%
32	13.324	1885	1887	1899	rVV5	16782	48585	6.97%	1.439%
33	13.428	1899	1904	1910	rVV	79764	139121	19.96%	4.121%
34	13.483	1910	1913	1920	rVB2	13137	24606	3.53%	0.729%
35	13.550	1920	1924	1929	rVB7	5150	10940	1.57%	0.324%
36	13.641	1930	1939	1944	rBV9	6675	17697	2.54%	0.524%

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37	13.757	1952	1958	1965	rVB3	35083	56866	8.16%	1.685%
38	13.964	1986	1992	1999	rVB2	37512	66319	9.52%	1.965%
39	14.196	2026	2030	2035	rVB5	6070	10076	1.45%	0.298%
40	14.611	2094	2098	2104	rVB2	10393	15713	2.25%	0.465%
41	15.208	2191	2196	2205	rBV8	3128	8642	1.24%	0.256%
42	15.385	2220	2225	2230	rBV	14440	26835	3.85%	0.795%
43	15.434	2230	2233	2238	rVB2	6220	9598	1.38%	0.284%

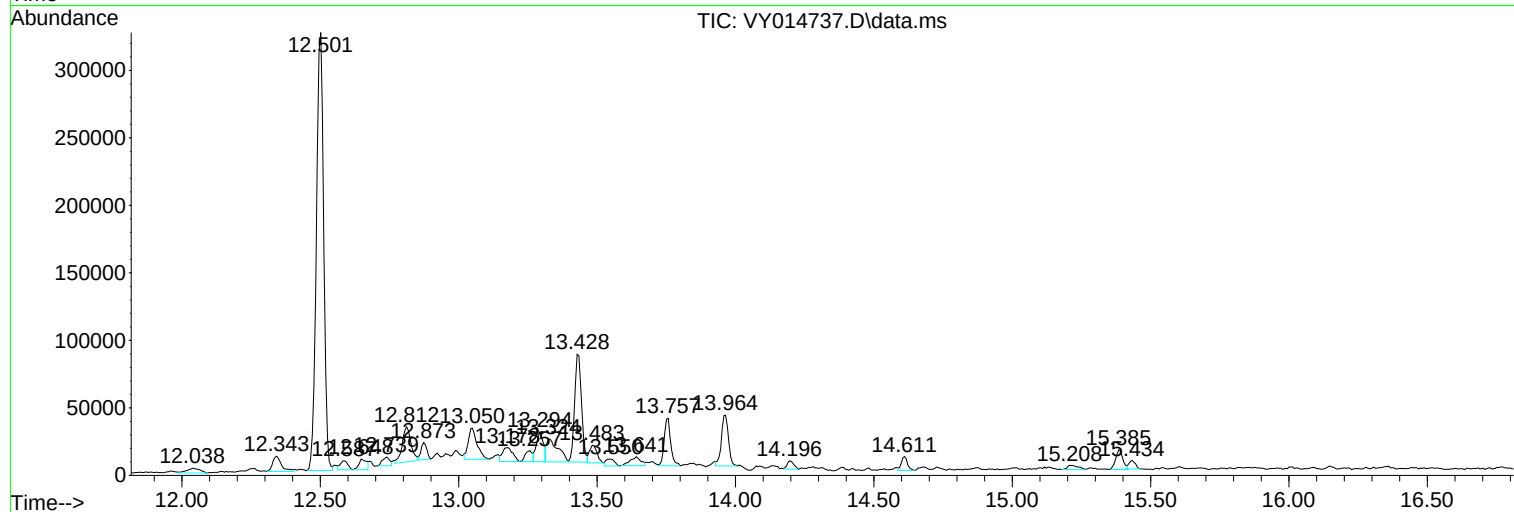
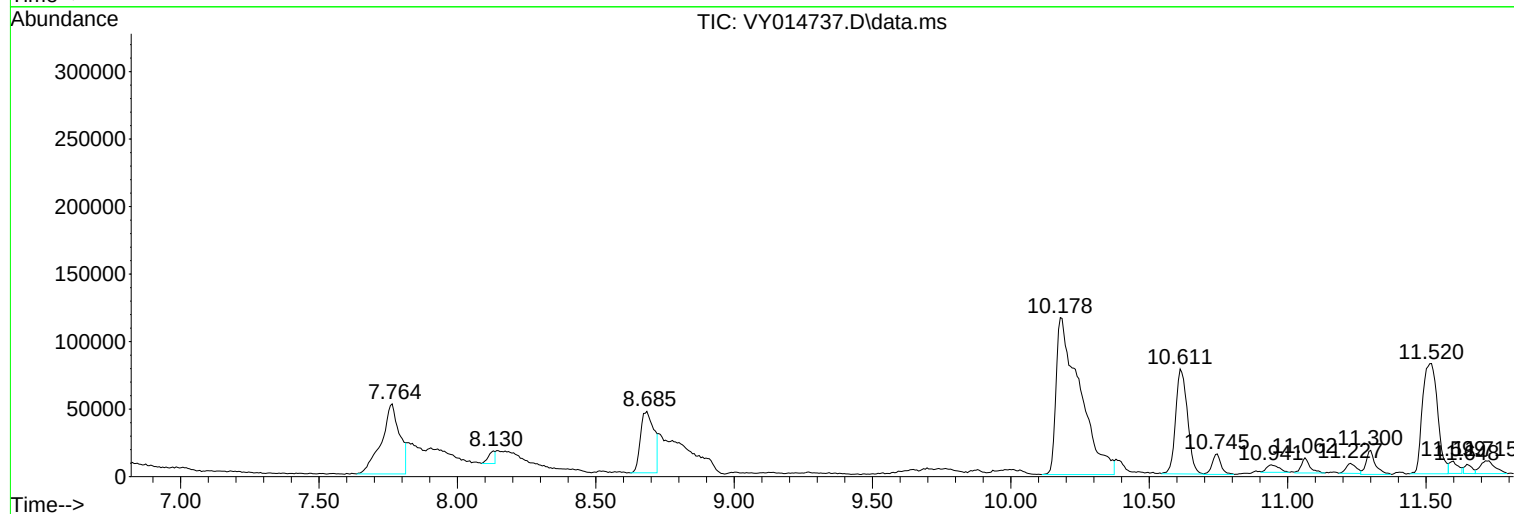
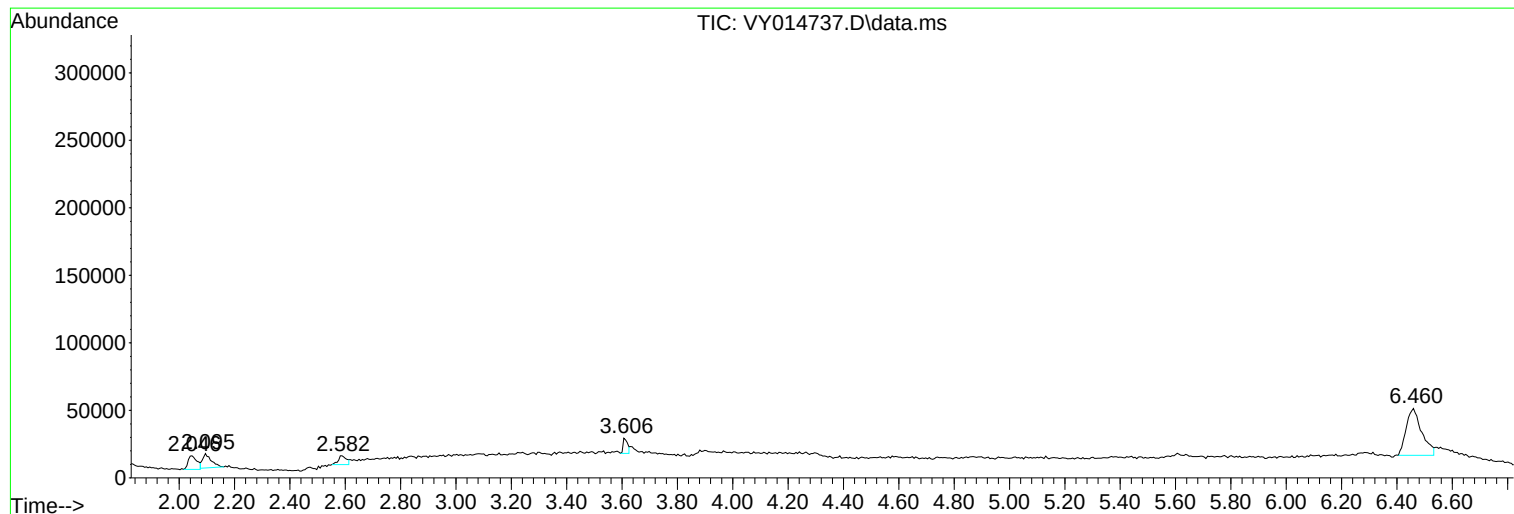
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071323S.M
Quant Title : SW846 8260

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



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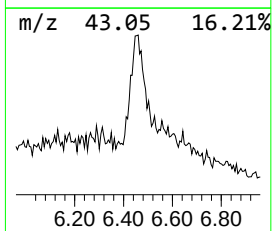
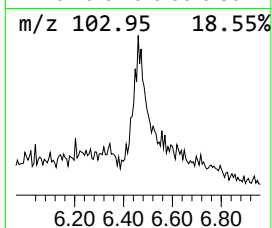
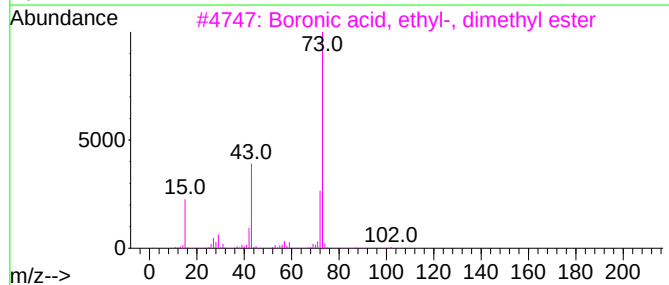
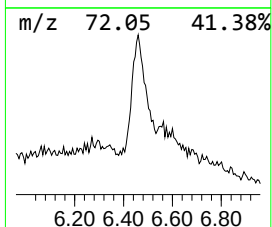
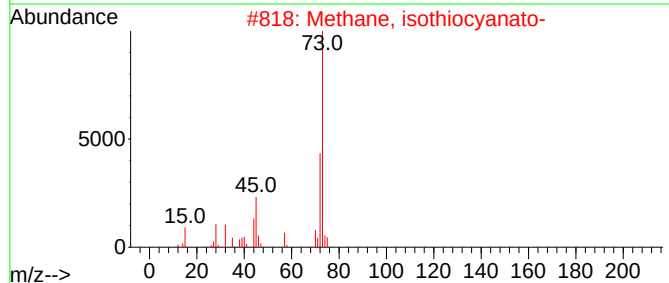
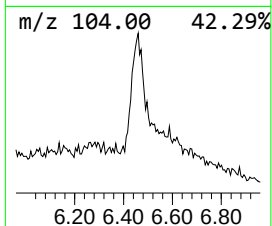
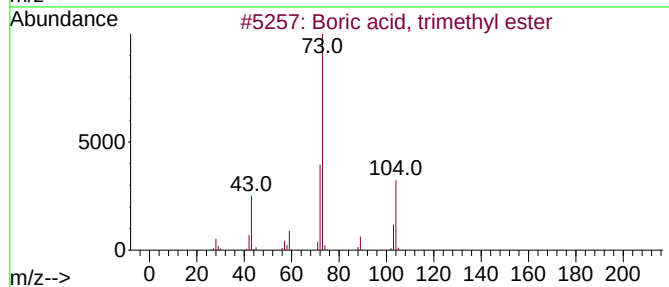
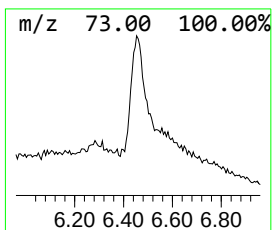
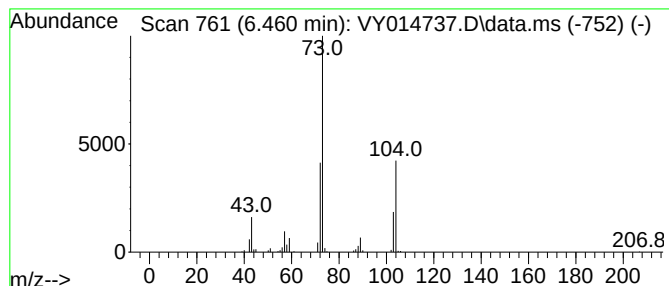
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071323S.M
Quant Title : SW846 8260

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

Peak Number 1 Boric acid, trimethyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.460	28.23 ug/l	135344	Pentafluorobenzene	7.764

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Boric acid, trimethyl ester	104	C3H9B03	000121-43-7	87
2			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
3			Boronic acid, ethyl-, dimethyl e...	102	C4H11B02	007318-82-3	9
4			1-Propanamine, 3-methoxy-	89	C4H11NO	005332-73-0	9
5			Guanidine, methyl-	73	C2H7N3	000471-29-4	5



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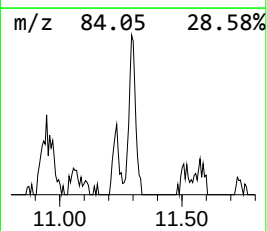
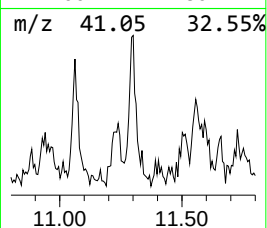
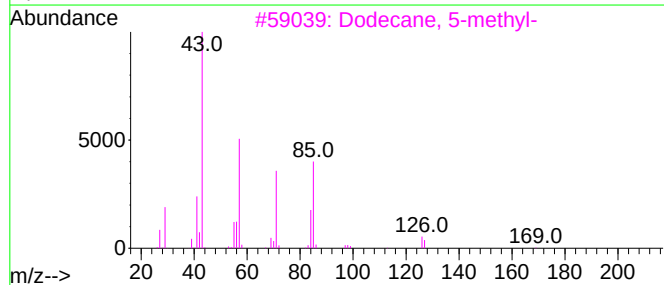
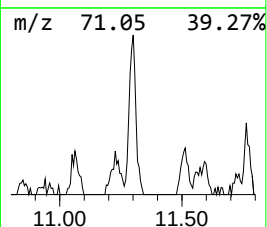
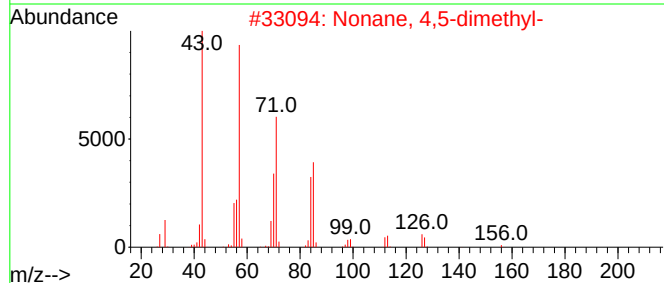
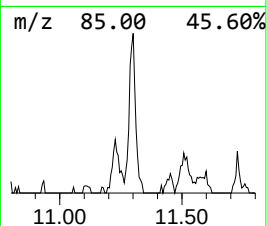
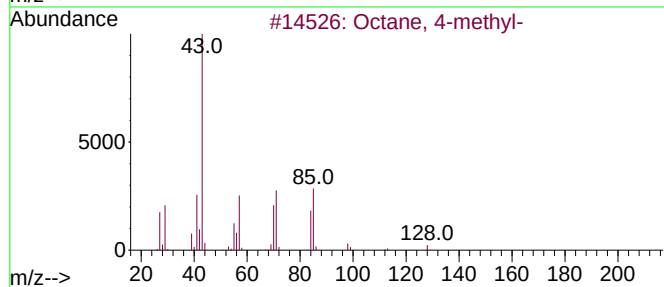
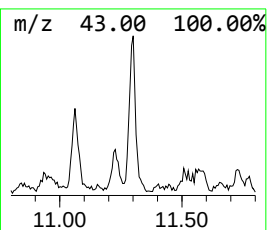
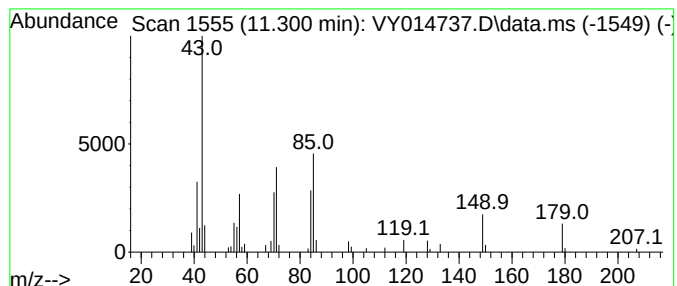
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octane, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.300	6.45 ug/l	40424	Chlorobenzene-d5	11.520

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 4-methyl-	128	C9H20	002216-34-4	81
2			Nonane, 4,5-dimethyl-	156	C11H24	017302-23-7	59
3			Dodecane, 5-methyl-	184	C13H28	017453-93-9	50
4			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	50
5			Hexane, 3-ethyl-	114	C8H18	000619-99-8	47



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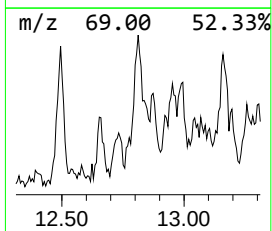
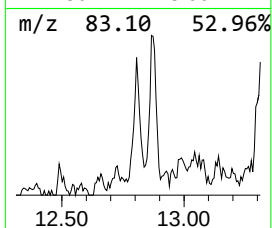
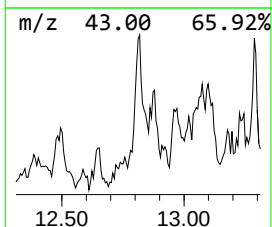
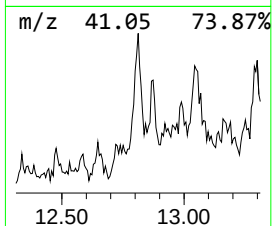
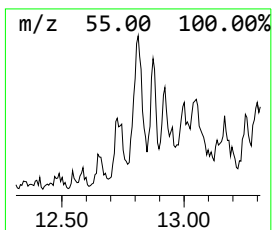
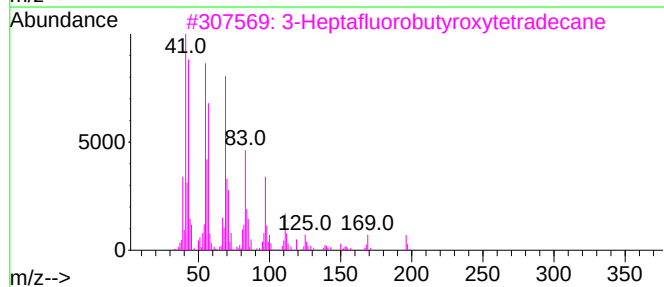
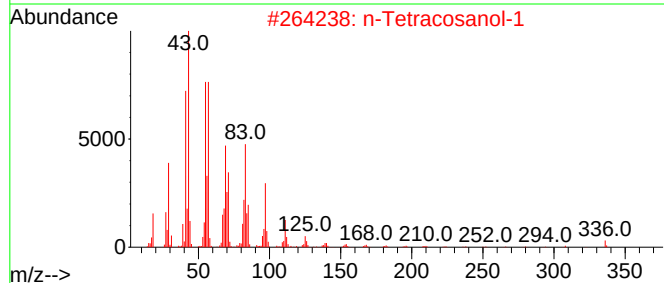
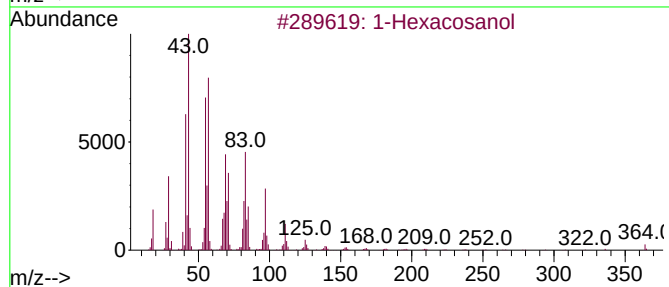
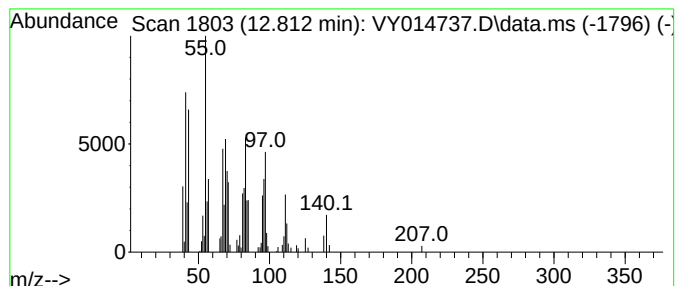
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Peak Number 4 1-Hexacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.812	20.53 ug/l	57123	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexacosanol	382	C26H54O	000506-52-5	52
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	52
3			3-Heptafluorobutyroxytetradecane	410	C18H29F7O2	1000245-49-8	47
4			1-Hexadecanol	242	C16H34O	036653-82-4	46
5			Cyclohexane, nonadecyl-	350	C25H50	022349-03-7	43



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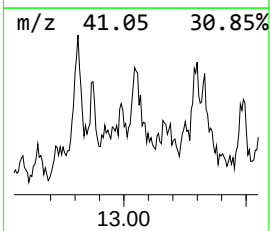
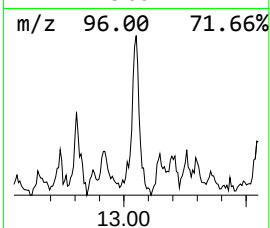
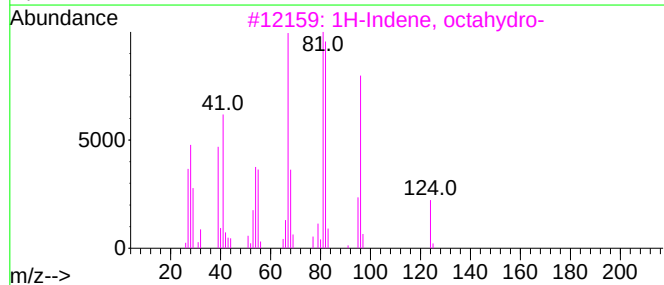
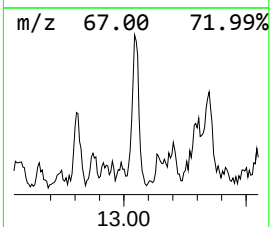
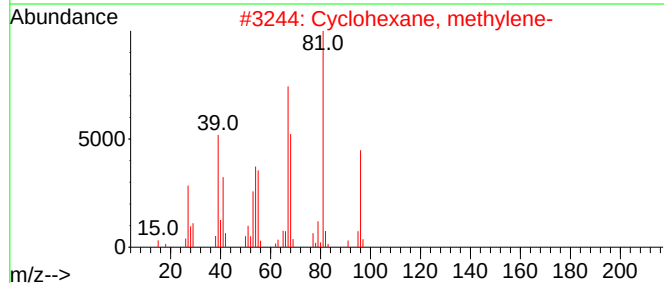
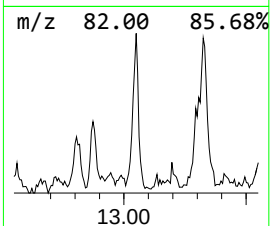
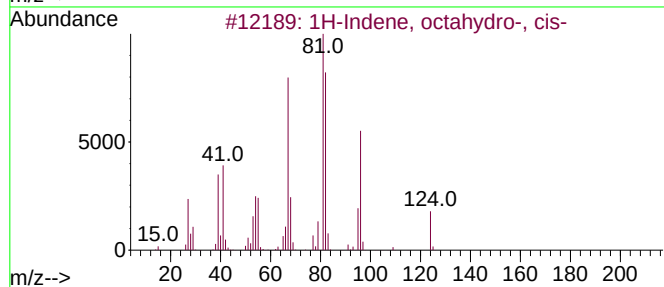
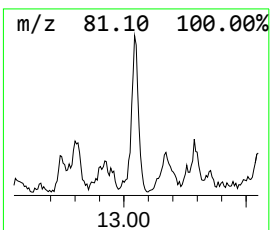
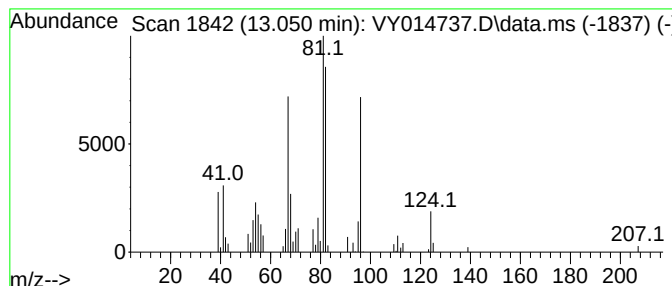
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TIC Integration Parameters: LSCINT.P

Peak Number 5 1H-Indene, octahydro-, cis- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.050	18.46 ug/l	51358	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, octahydro-, cis-	124	C9H16	004551-51-3	94
2			Cyclohexane, methylene-	96	C7H12	001192-37-6	58
3			1H-Indene, octahydro-	124	C9H16	000496-10-6	53
4			Carbonic acid, ethyl cyclohexylm...	186	C10H18O3	1000357-91-5	50
5			Carbonic acid, propyl cyclohexyl...	200	C11H20O3	1000357-81-6	50



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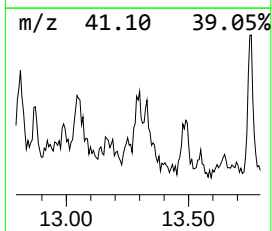
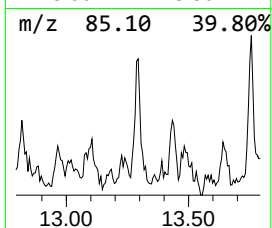
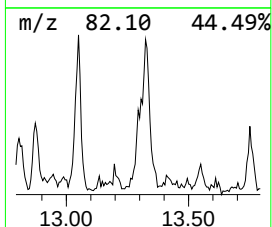
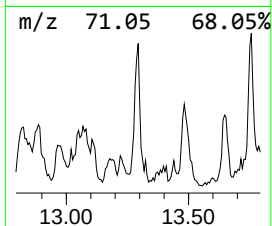
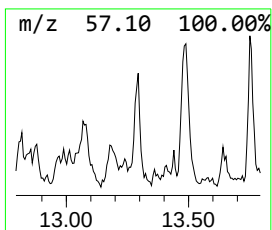
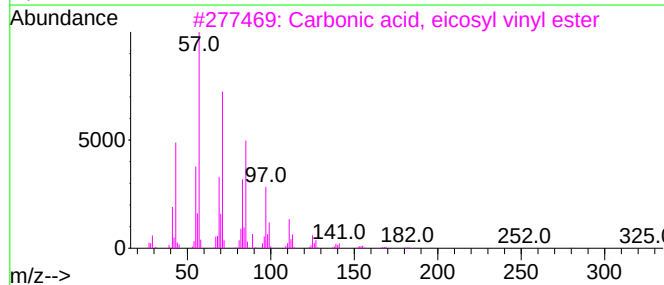
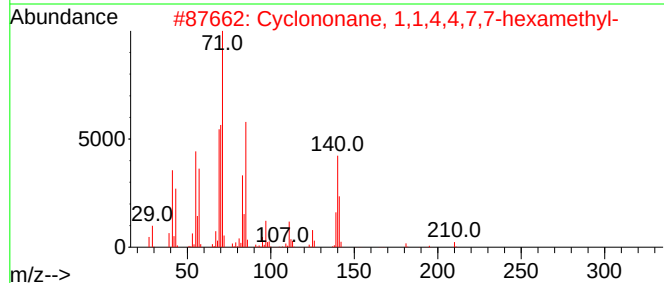
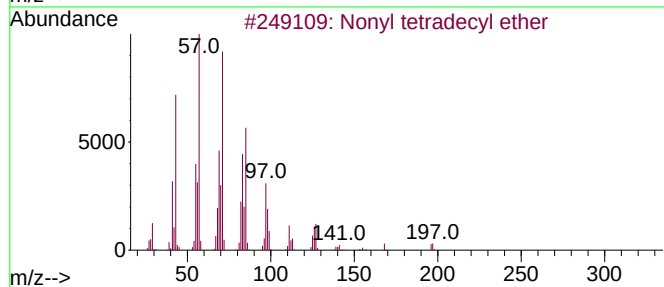
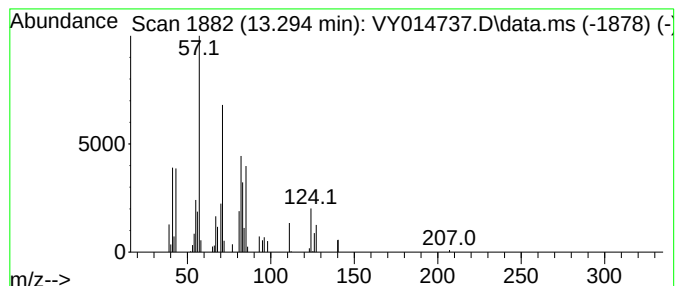
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Quant Title : SW846 8260

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

Peak Number 6 Nonyl tetradecyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.294	13.97 ug/l	38879	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonyl tetradecyl ether	340	C23H48O	1000406-37-6	58
2			Cyclononane, 1,1,4,4,7,7-hexamet...	210	C15H30	149331-19-1	50
3			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	47
4			Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	43
5			Carbonic acid, tridecyl vinyl ester	270	C16H30O3	1000382-54-7	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY072123\
Data File : VY014737.D
Acq On : 21 Jul 2023 11:23
Operator : SY/MD
Sample : 03681-08
Misc : 2.38g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RPTP-3-GRAB-5

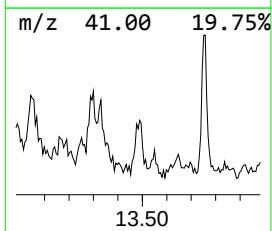
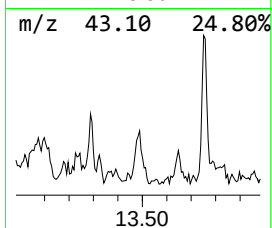
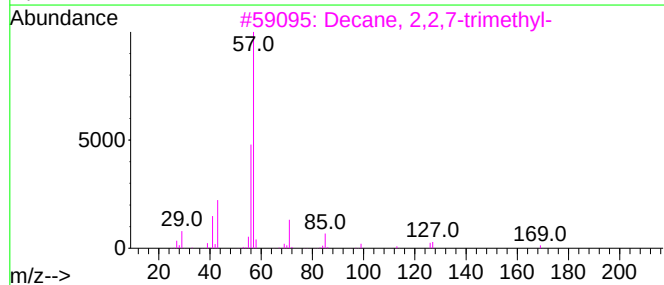
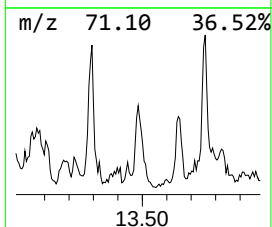
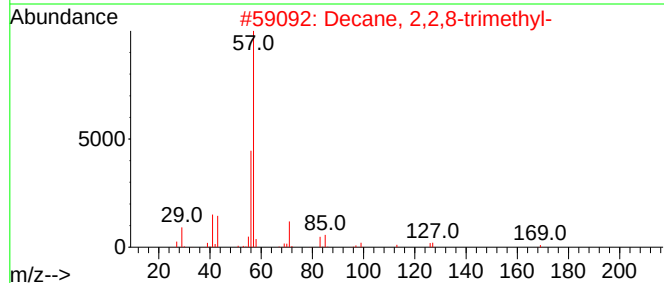
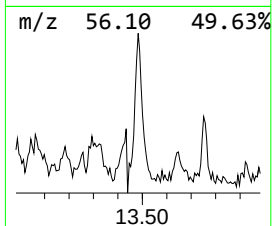
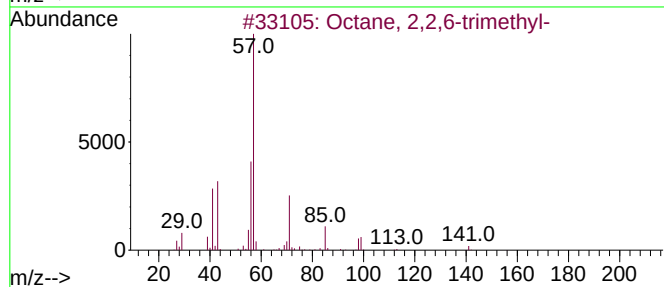
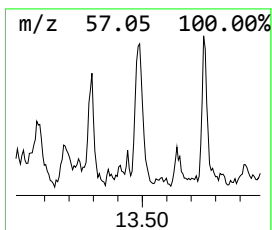
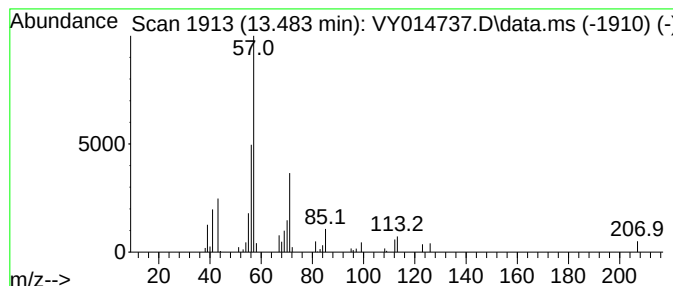
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Quant Title : SW846 8260

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

Peak Number 7 Octane, 2,2,6-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.483	8.84 ug/l	24606	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	64
2			Decane, 2,2,8-trimethyl-	184	C13H28	062238-01-1	59
3			Decane, 2,2,7-trimethyl-	184	C13H28	062237-99-4	59
4			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	47
5			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY072123\
Data File : VY014737.D
Acq On : 21 Jul 2023 11:23
Operator : SY/MD
Sample : 03681-08
Misc : 2.38g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RPTP-3-GRAB-5

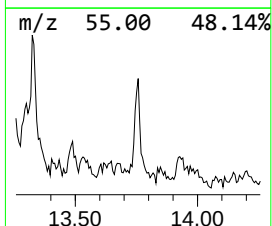
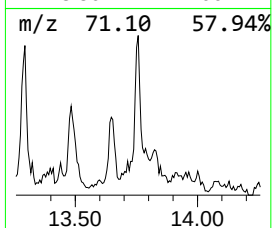
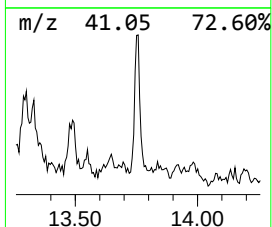
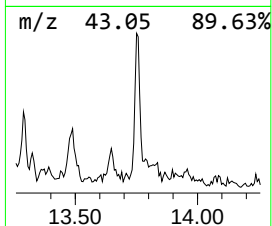
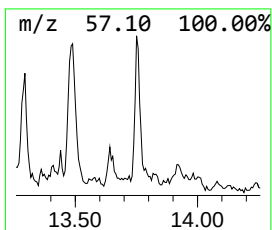
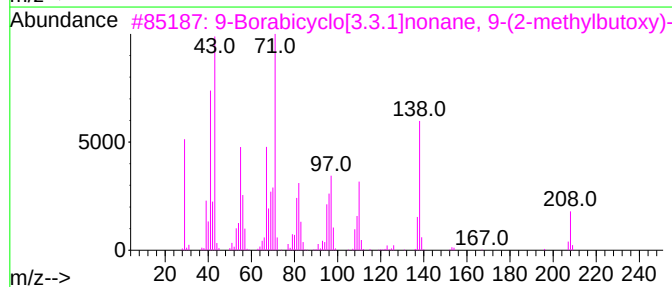
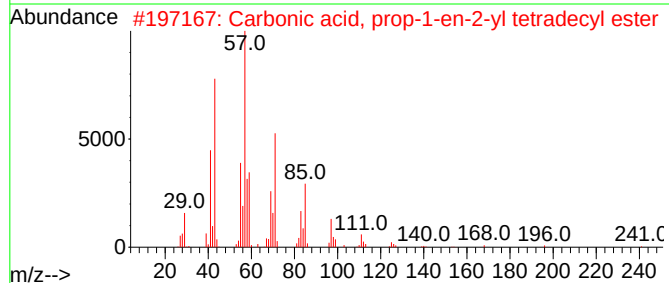
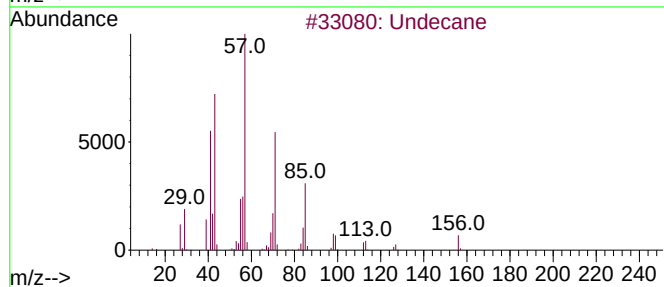
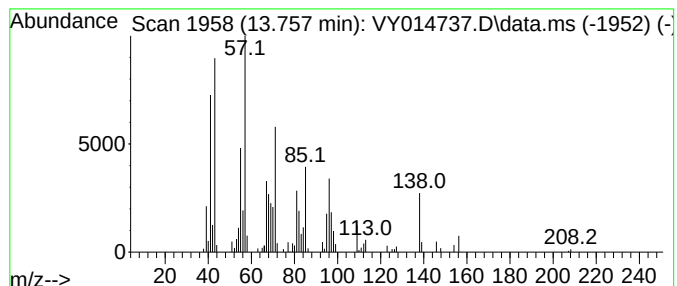
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Quant Title : SW846 8260

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

Peak Number 8 Undecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.757	20.44 ug/l	56866	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	78
2			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	58
3			9-Borabicyclo[3.3.1]nonane, 9-(2...	208	C13H25BO	094537-53-8	49
4			Hexadecane	226	C16H34	000544-76-3	47
5			Oxirane, tetradecyl-	240	C16H32O	007320-37-8	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY072123\
Data File : VY014737.D
Acq On : 21 Jul 2023 11:23
Operator : SY/MD
Sample : 03681-08
Misc : 2.38g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RPTP-3-GRAB-5

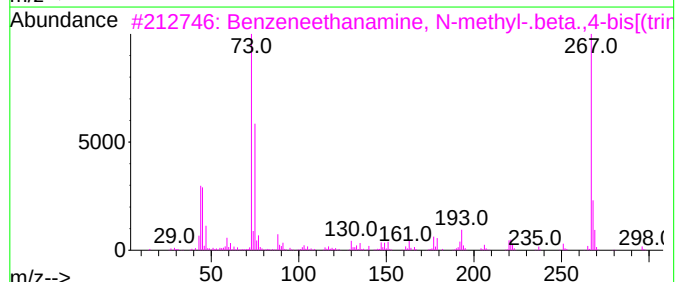
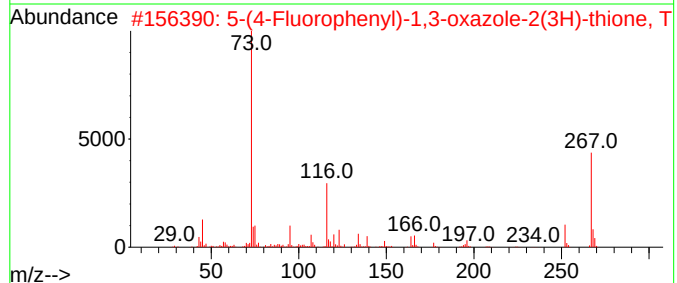
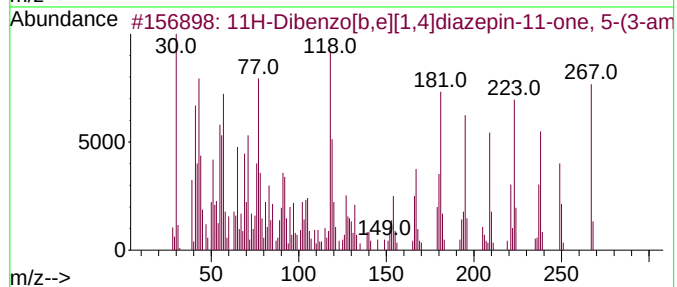
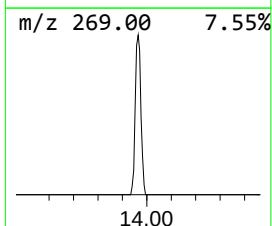
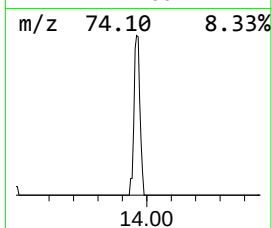
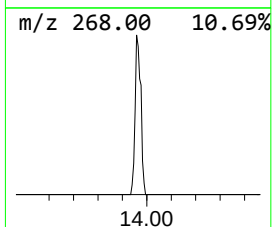
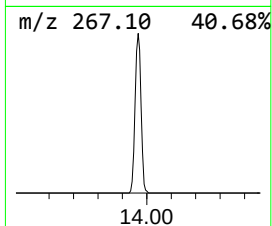
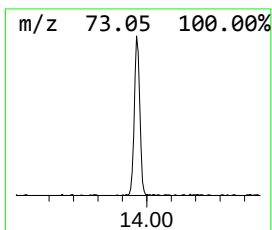
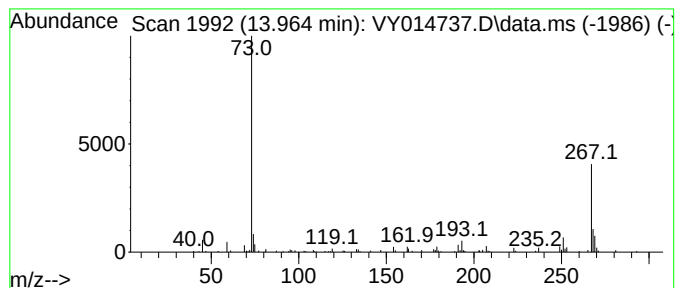
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071323S.M
Quant Title : SW846 8260

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

Peak Number 9 11H-Dibenzo[b,e][1,4]diazep... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.964	23.84 ug/l	66319	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Dibenzo[b,e][1,4]diazepin-11...	267	C16H17N3O	013450-73-2	53
2			5-(4-Fluorophenyl)-1,3-oxazole-2...	267	C12H14FNOSSi	1000497-07-6	45
3			Benzeneethanamine, N-methyl-.bet...	311	C15H29NO2Si2	029522-18-7	45
4			Benzeneethanamine, N-[(pentaflu...	475	C21H26F5NO2Si2	055429-85-1	43
5			Salicylic acid, 2TMS derivative	282	C13H22O3Si2	003789-85-3	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY072123\
Data File : VY014737.D
Acq On : 21 Jul 2023 11:23
Operator : SY/MD
Sample : 03681-08
Misc : 2.38g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RPTP-3-GRAB-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071323S.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
Boric acid, tri...	6.460	28.2	ug/l	135344	1	7.764	239747	50.0
Octane, 4-methyl-	11.300	6.5	ug/l	40424	3	11.520	313300	50.0
1-Hexacosanol	12.812	20.5	ug/l	57123	4	13.428	139121	50.0
1H-Indene, octa...	13.050	18.5	ug/l	51358	4	13.428	139121	50.0
Nonyl tetradecy...	13.294	14.0	ug/l	38879	4	13.428	139121	50.0
Octane, 2,2,6-t...	13.483	8.8	ug/l	24606	4	13.428	139121	50.0
Undecane	13.757	20.4	ug/l	56866	4	13.428	139121	50.0
11H-Dibenzo[b,e...	13.964	23.8	ug/l	66319	4	13.428	139121	50.0