

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071122\
 Data File : VY009507.D
 Acq On : 11 Jul 2022 14:03
 Operator : KP/MD
 Sample : N3593-14
 Misc : 6.15g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 20220492B-10B

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\82Y070722S.M
 Title : SW846 8260

Signal : TIC: VY009507.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.857	3	6	13	rVB2	4807	7251	1.32%	0.198%
2	3.936	340	347	356	rBV2	8231	21662	3.94%	0.590%
3	4.180	377	387	401	rBV	29070	80933	14.73%	2.206%
4	4.704	463	473	486	rVB2	19596	57612	10.49%	1.570%
5	5.741	633	643	653	rVB5	3948	12178	2.22%	0.332%
6	6.978	837	846	853	rBV4	3602	10650	1.94%	0.290%
7	7.710	955	966	972	rBV	77238	183658	33.43%	5.006%
8	7.783	972	978	989	rVB	165894	377934	68.80%	10.302%
9	8.136	1028	1036	1046	rBV	63410	138490	25.21%	3.775%
10	8.685	1118	1126	1137	rBV	254820	495841	90.26%	13.516%
11	10.173	1363	1370	1378	rBV	211894	381806	69.50%	10.408%
12	11.489	1579	1586	1595	rBV	330631	549322	100.00%	14.974%
13	11.703	1612	1621	1625	rBV6	4609	13468	2.45%	0.367%
14	12.008	1662	1671	1674	rBV9	7584	19994	3.64%	0.545%
15	12.203	1697	1703	1704	rBV6	4711	7409	1.35%	0.202%
16	12.233	1704	1708	1713	rVB6	6539	12077	2.20%	0.329%
17	12.300	1713	1719	1720	rBV5	4843	7780	1.42%	0.212%
18	12.483	1741	1749	1757	rBV2	275464	499352	90.90%	13.612%
19	12.562	1757	1762	1767	rVV9	4363	8295	1.51%	0.226%
20	12.806	1793	1802	1814	rVB9	11866	41243	7.51%	1.124%
21	12.910	1814	1819	1823	rBV2	33660	54247	9.88%	1.479%
22	13.044	1836	1841	1842	rBV5	6663	9257	1.69%	0.252%
23	13.172	1858	1862	1865	rBV5	5498	9790	1.78%	0.267%
24	13.282	1876	1880	1885	rBV2	13511	18516	3.37%	0.505%
25	13.422	1896	1903	1909	rBV	257211	403122	73.39%	10.989%
26	13.471	1909	1911	1917	rVB3	12878	19751	3.60%	0.538%
27	13.751	1950	1957	1961	rBV9	12188	31985	5.82%	0.872%
28	13.959	1987	1991	1998	rVB2	25678	42078	7.66%	1.147%
29	14.074	2008	2010	2015	rVB5	10562	13543	2.47%	0.369%
30	14.135	2015	2020	2025	rBV9	7789	18357	3.34%	0.500%
31	14.202	2028	2031	2035	rBV6	7172	10437	1.90%	0.284%
32	14.257	2035	2040	2051	rBV9	11951	41098	7.48%	1.120%
33	14.385	2059	2061	2064	rBV4	5383	7941	1.45%	0.216%
34	14.684	2105	2110	2113	rBV6	9863	18231	3.32%	0.497%
35	14.733	2114	2118	2123	rVB8	13034	23665	4.31%	0.645%
36	14.940	2148	2152	2156	rVB7	12017	19577	3.56%	0.534%

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ClientSampleId :
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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\82Y070722S.M
Title : SW846 8260

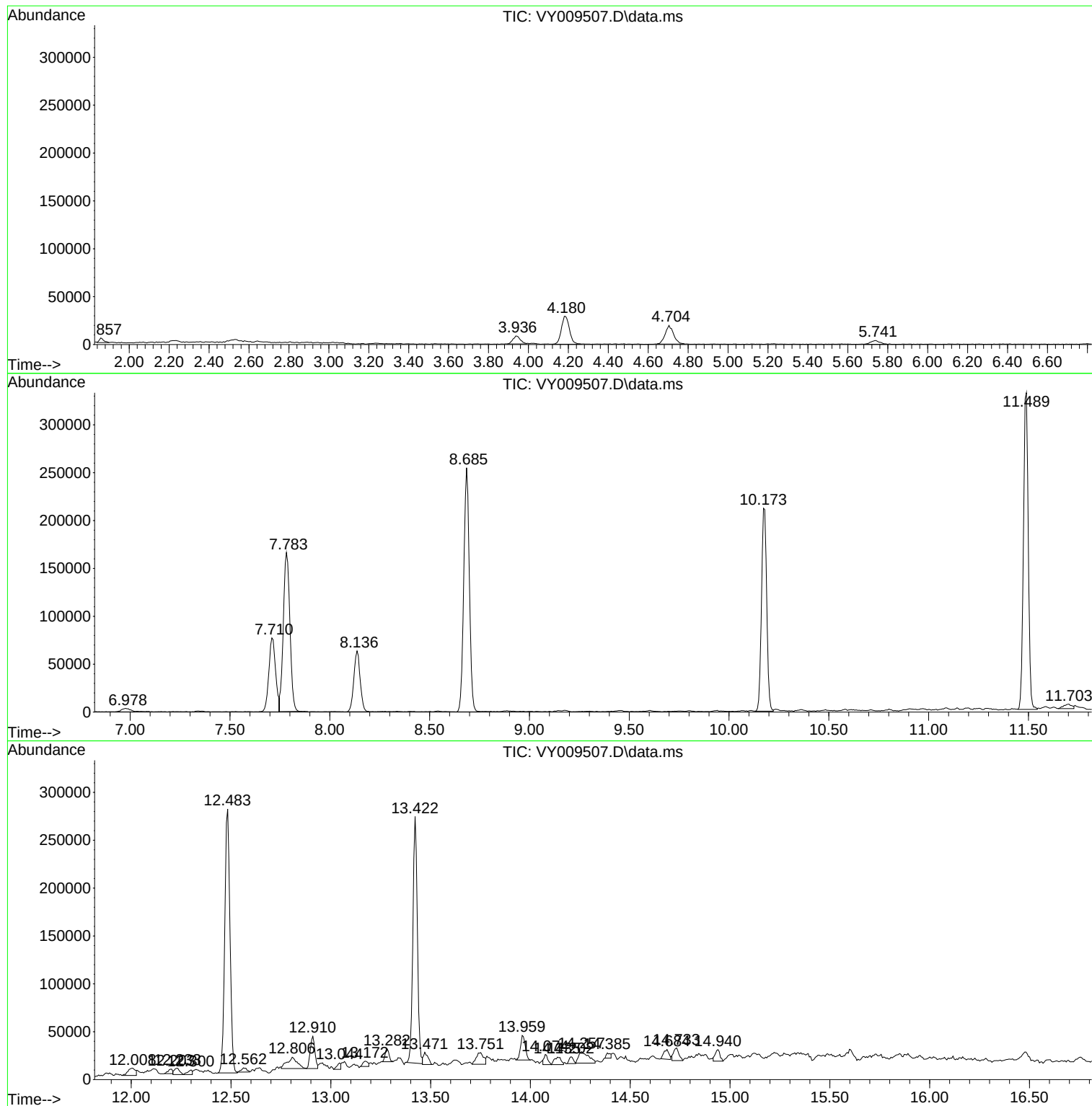
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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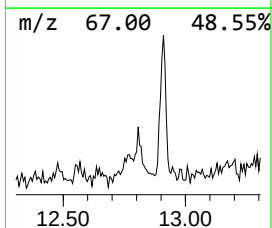
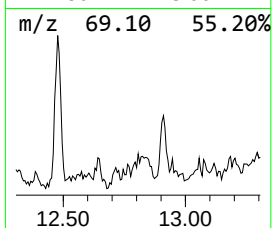
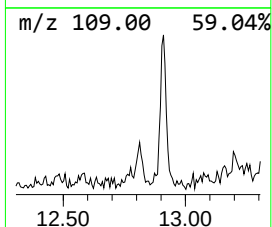
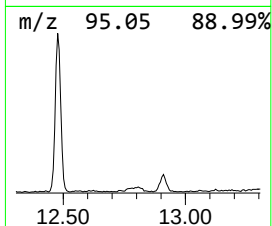
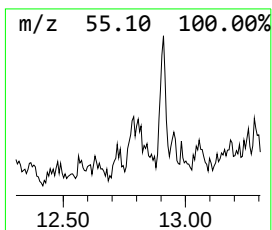
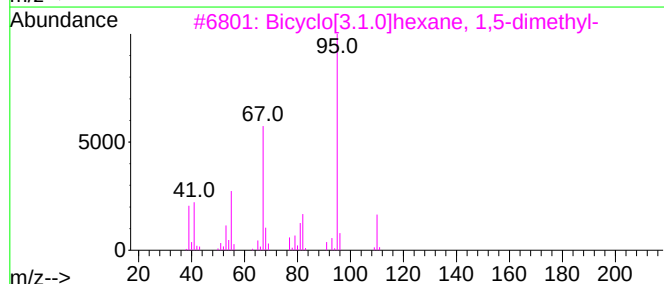
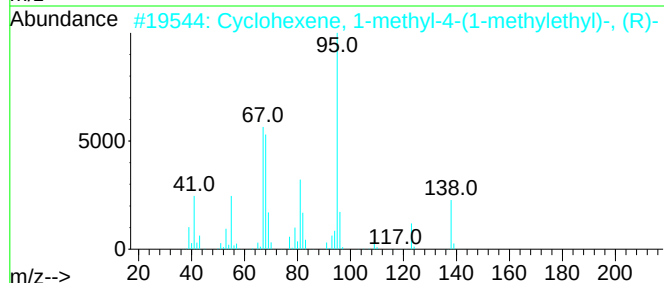
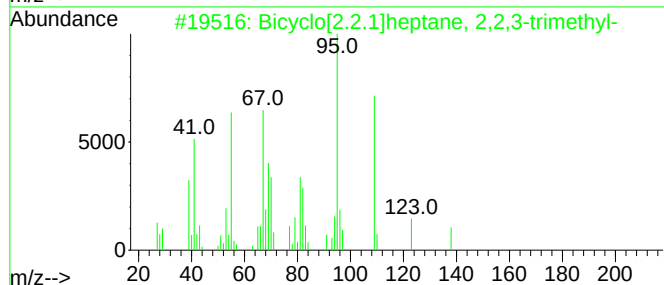
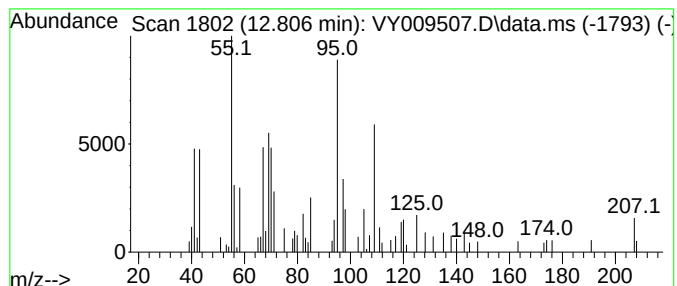
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070722S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown12.806 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.806	5.12 ug/l	41243	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	38
2			Cyclohexene, 1-methyl-4-(1-methy...	138	C10H18	001195-31-9	27
3			Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	27
4			5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	27
5			2(1H)-Pyridinone	95	C5H5NO	000142-08-5	27



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Instrument :
MSVOA_Y
ClientSampleId :
20220492B-10B

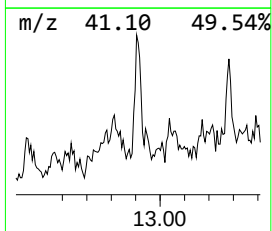
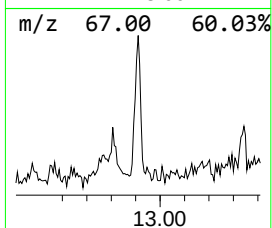
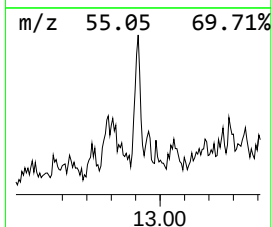
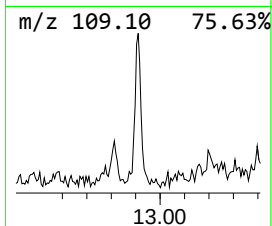
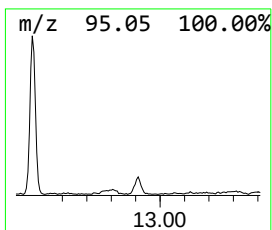
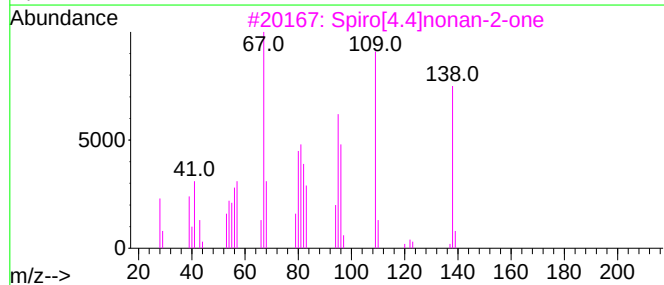
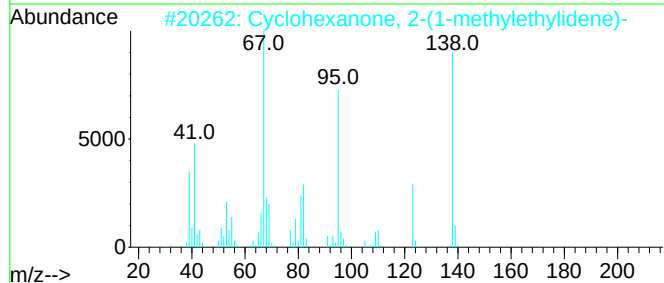
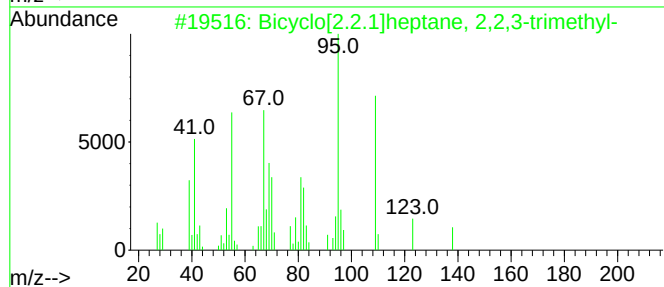
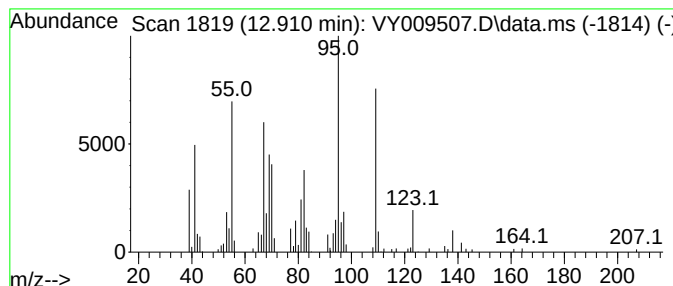
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070722S.M
Quant Title : SW846 8260

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

Peak Number 3 Bicyclo[2.2.1]heptane, 2,2,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.910	6.73 ug/l	54247	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	94
2			Cyclohexanone, 2-(1-methylethylidene)	138	C9H14O	013747-73-4	55
3			Spiro[4.4]nonan-2-one	138	C9H14O	034177-18-9	49
4			Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	49
5			1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	46



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20220492B-10B

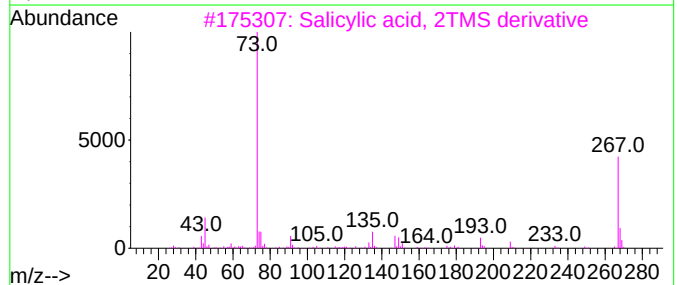
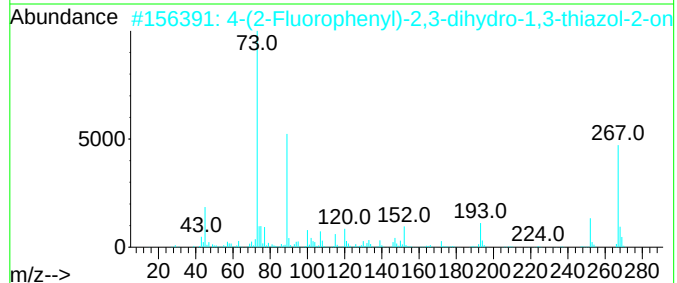
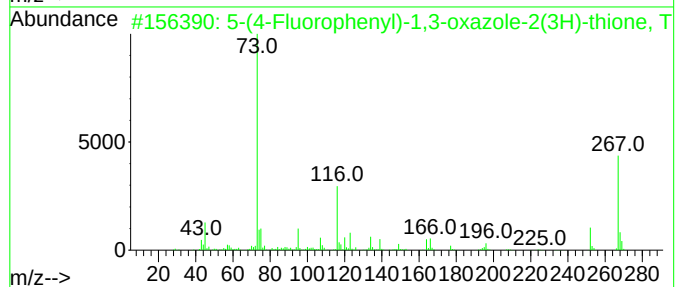
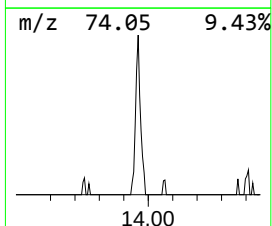
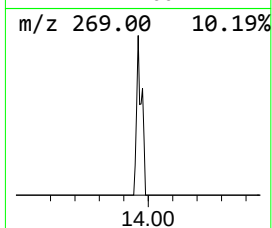
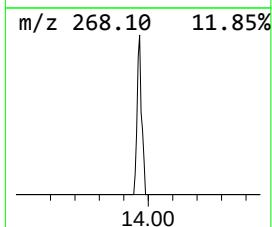
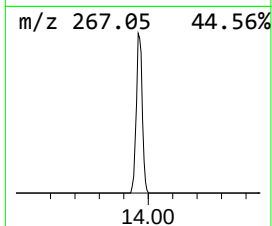
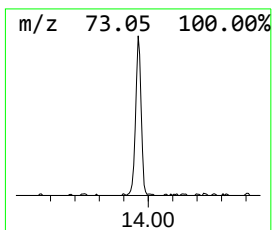
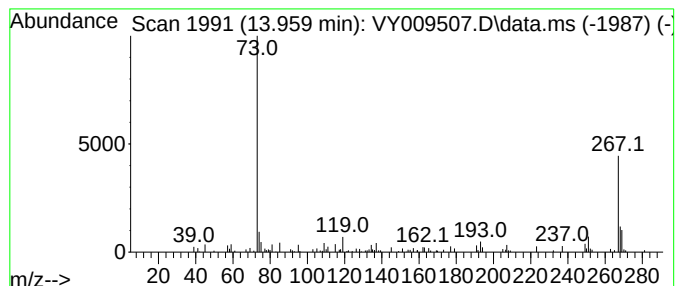
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Quant Title : SW846 8260

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

Peak Number 4 5-(4-Fluorophenyl)-1,3-oxaz... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.959	5.22 ug/l	42078	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-(4-Fluorophenyl)-1,3-oxazole-2...	267	C12H14FNOSSi	1000497-07-6	59
2			4-(2-Fluorophenyl)-2,3-dihydro-1...	267	C12H14FNOSSi	1000504-37-6	53
3			Salicylic acid, 2TMS derivative	282	C13H22O3Si2	003789-85-3	53
4			Acridone, TMS derivative	267	C16H17NOSi	1000478-16-0	38
5			Benzeneethanamine, N-[(pentaflu...	475	C21H26F5NO2Si2	055429-85-1	38



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ClientSampleId :
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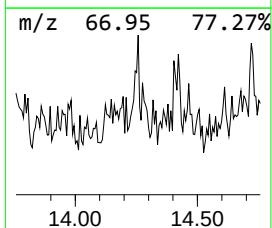
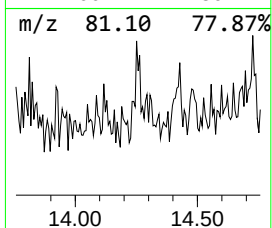
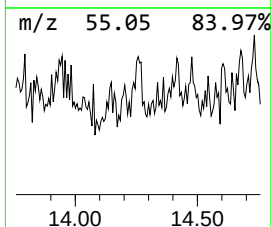
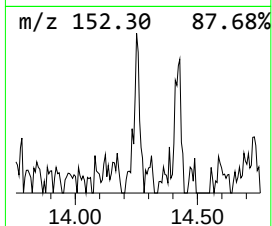
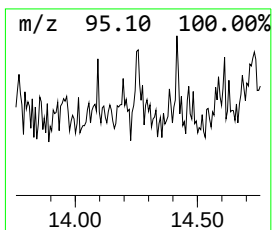
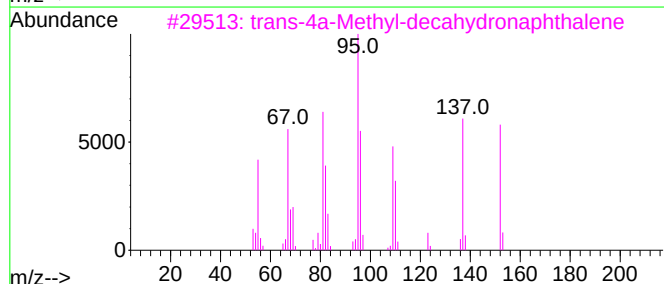
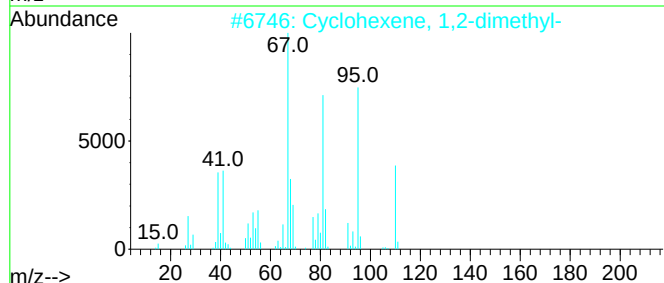
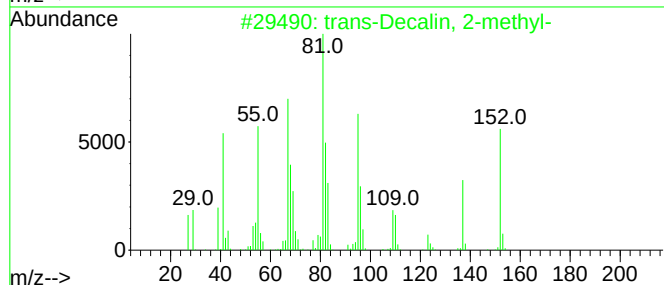
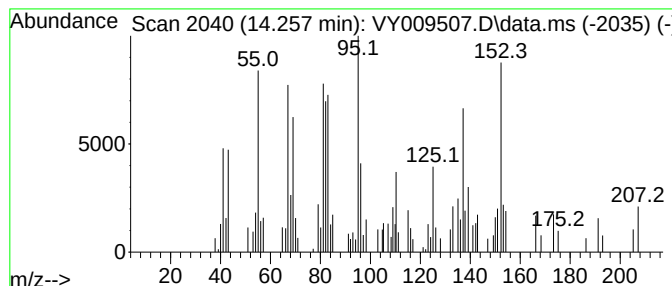
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 trans-Decalin, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.257	5.10 ug/l	41098	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	60
2			Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	55
3			trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	52
4			cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	49
5			1-Adamantanol	152	C10H16O	000768-95-6	46



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown12.806	12.806	5.1	ug/l	41243	4	13.422	403122	50.0
Bicyclo[2.2.1]h...	12.910	6.7	ug/l	54247	4	13.422	403122	50.0
5-(4-Fluorophen...	13.959	5.2	ug/l	42078	4	13.422	403122	50.0
trans-Decalin, ...	14.257	5.1	ug/l	41098	4	13.422	403122	50.0