

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY080522\
 Data File : VY009871.D
 Acq On : 05 Aug 2022 23:17
 Operator : KP/MD
 Sample : N4062-01
 Misc : 5.02g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 OK-02-080422

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\82Y080322S.M
 Title : SW846 8260

Signal : TIC: VY009871.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.698	463	472	484	rBB4	3873	11522	2.95%	0.721%
2	5.728	633	641	654	rVB4	7229	22893	5.87%	1.432%
3	6.972	835	845	861	rBV	9380	28738	7.36%	1.797%
4	7.710	958	966	971	rBV	20318	45789	11.73%	2.864%
5	7.783	971	978	987	rVB2	41144	92246	23.64%	5.769%
6	8.124	1021	1034	1046	rVB3	30331	99657	25.54%	6.232%
7	8.685	1118	1126	1137	rVB	76526	147972	37.92%	9.254%
8	10.173	1363	1370	1378	rBV	84684	151555	38.84%	9.478%
9	10.575	1432	1436	1442	rBV2	5675	8974	2.30%	0.561%
10	10.947	1491	1497	1503	rBV2	8298	15305	3.92%	0.957%
11	11.313	1553	1557	1564	rVB3	6206	10045	2.57%	0.628%
12	11.483	1579	1585	1593	rBV	134318	224739	57.59%	14.054%
13	12.093	1671	1685	1687	rBV8	20066	71270	18.26%	4.457%
14	12.477	1743	1748	1757	rBV2	80497	129880	33.28%	8.122%
15	13.184	1854	1864	1869	rBV10	14280	48081	12.32%	3.007%
16	13.422	1891	1903	1916	rVB	179249	390219	100.00%	24.403%
17	13.757	1951	1958	1959	rBV6	10836	22448	5.75%	1.404%
18	15.318	2210	2214	2220	rVB3	9411	18607	4.77%	1.164%
19	15.477	2234	2240	2251	rVB6	17981	59116	15.15%	3.697%

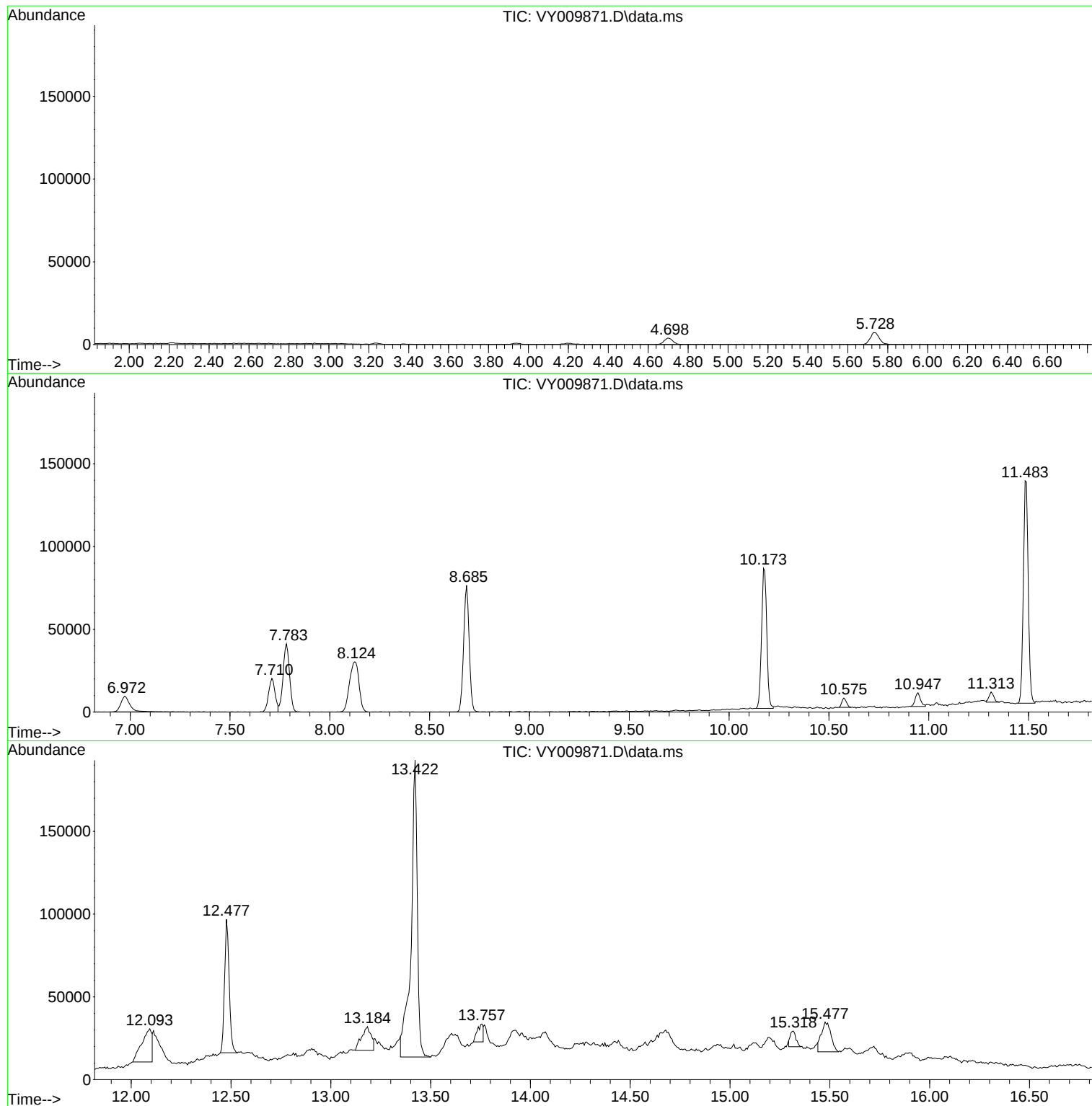
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Quant Title : SW846 8260

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



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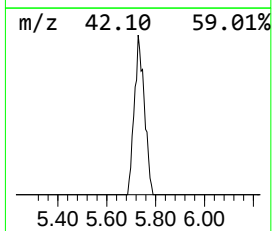
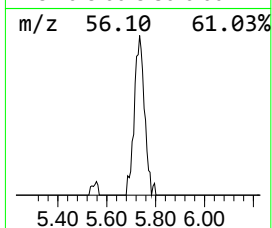
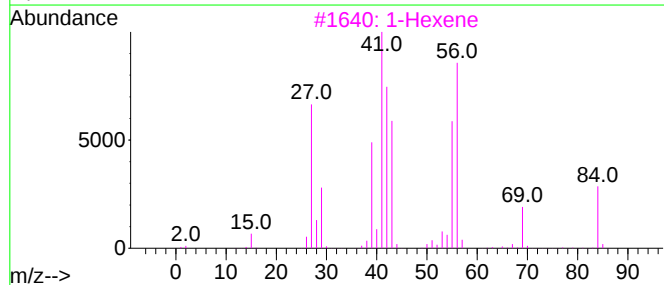
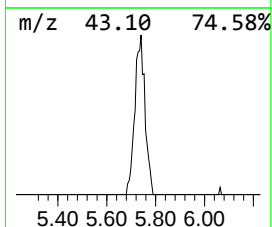
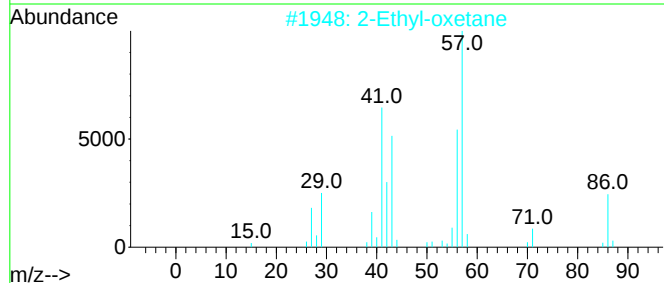
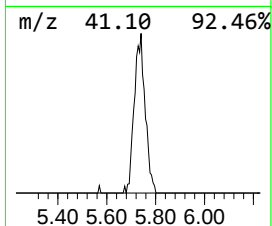
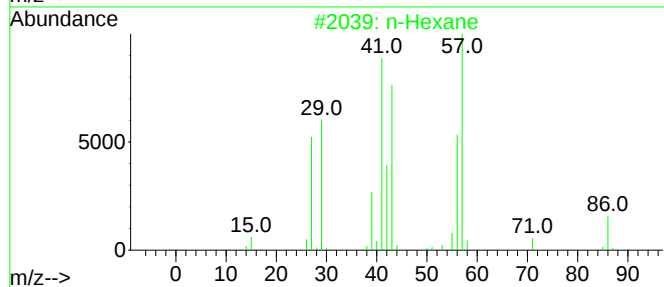
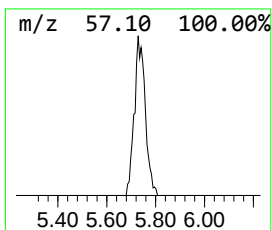
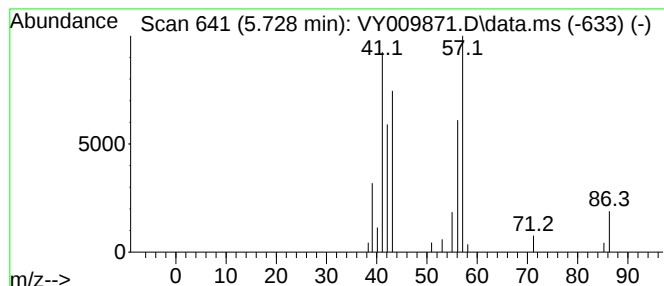
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y080322S.M
Quant Title : SW846 8260

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

Peak Number 2 n-Hexane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.728	12.41 ug/l	22893	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexane	86	C6H14	000110-54-3	72
2			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	50
3			1-Hexene	84	C6H12	000592-41-6	42
4			Hexane, 2-chloro-	120	C6H13Cl	000638-28-8	33
5			Cyclobutane	56	C4H8	000287-23-0	27



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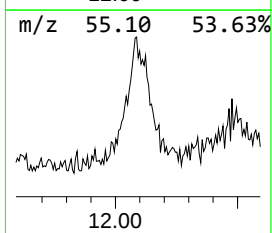
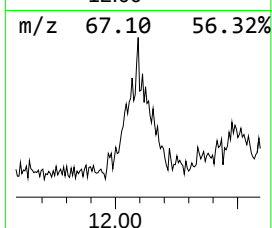
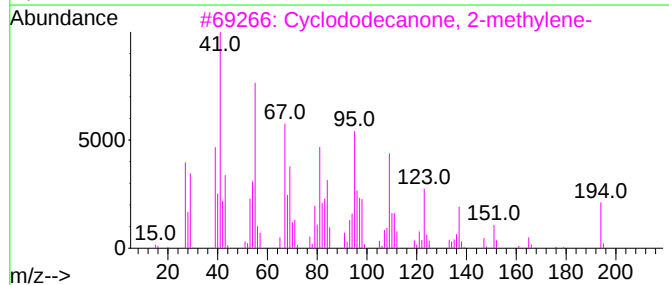
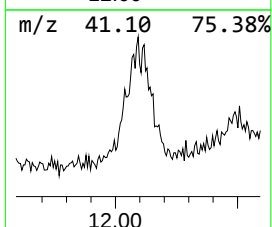
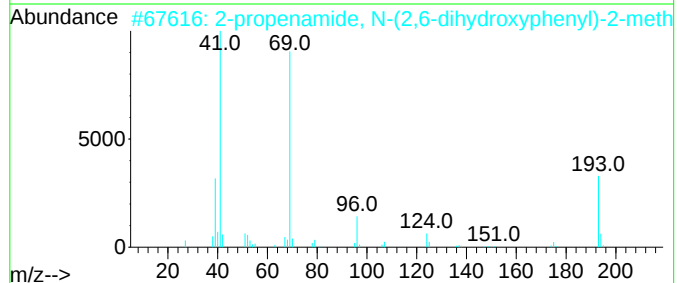
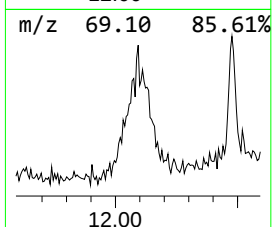
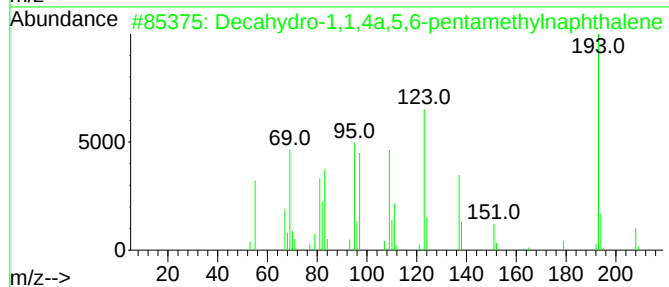
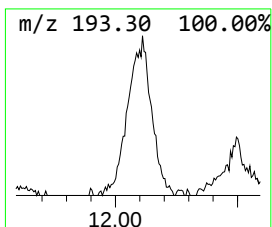
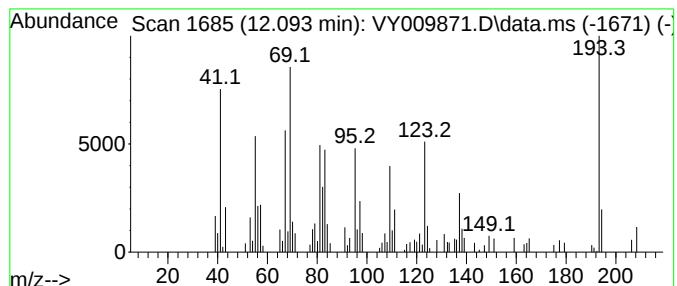
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ClientSampleId :
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Peak Number 4 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.093	15.86 ug/l	71270	Chlorobenzene-d5	11.489	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	86
2	2-propenamide, N-(2,6-dihydroxyp...	193	C10H11NO3	1000395-98-7	38
3	Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	35
4	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	35
5	Citronellol	156	C10H20O	000106-22-9	27



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Instrument :
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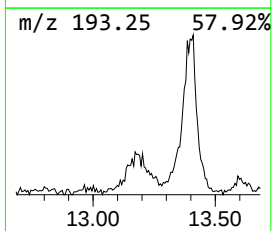
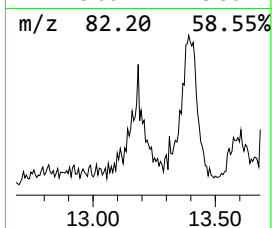
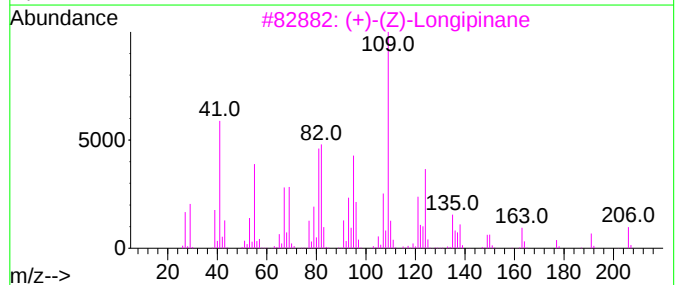
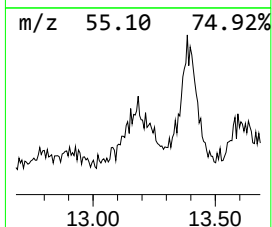
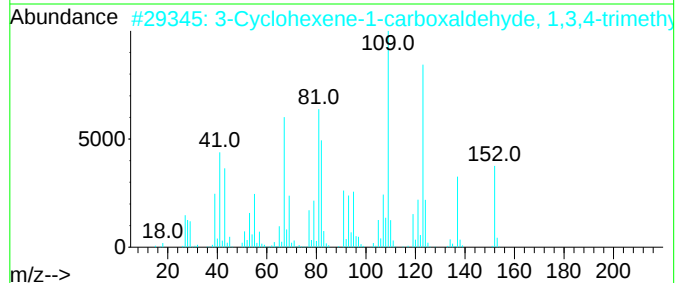
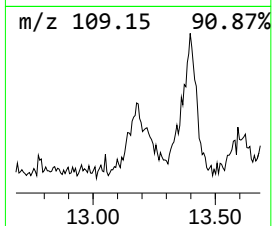
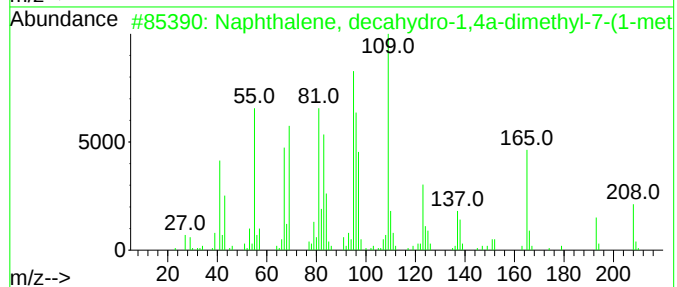
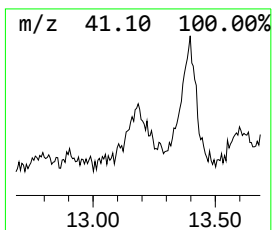
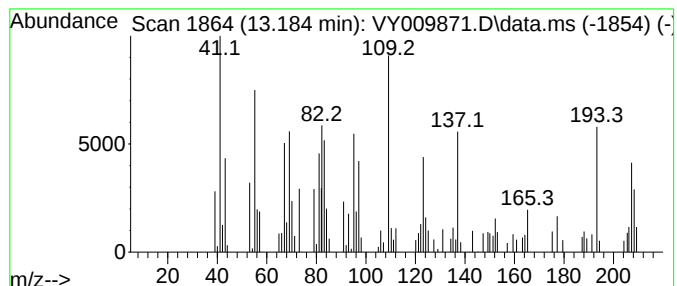
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Peak Number 5 unknown13.184 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.184	6.16 ug/l	48081	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-1,4a-dime...	208	C15H28	030824-81-8	38
2			3-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	040702-26-9	25
3			(+)-(Z)-Longipinane	206	C15H26	1000156-12-3	20
4			6,6-Dimethyl-cyclooct-4-enone	152	C10H16O	1000194-10-0	18
5			Longipinane, (E)-	206	C15H26	1000156-14-5	18



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Instrument :
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ClientSampleId :
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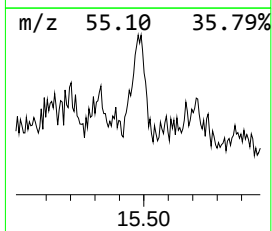
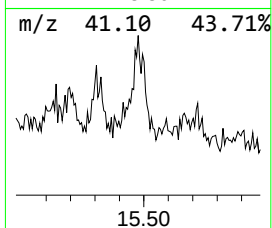
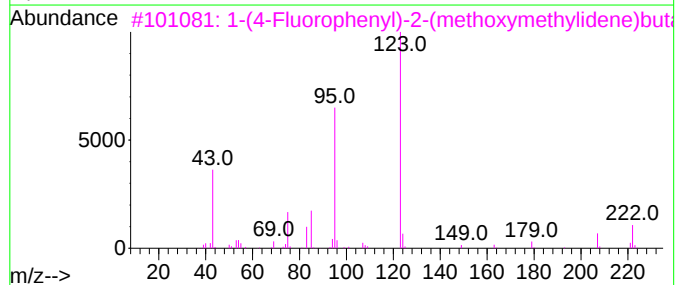
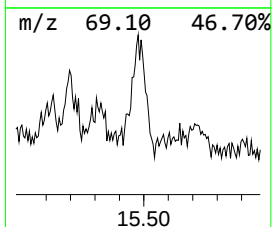
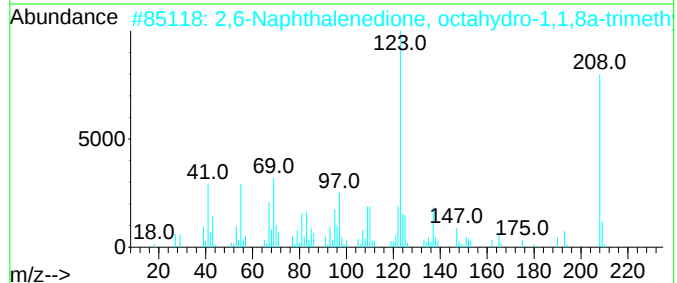
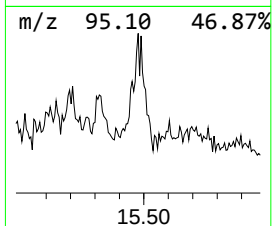
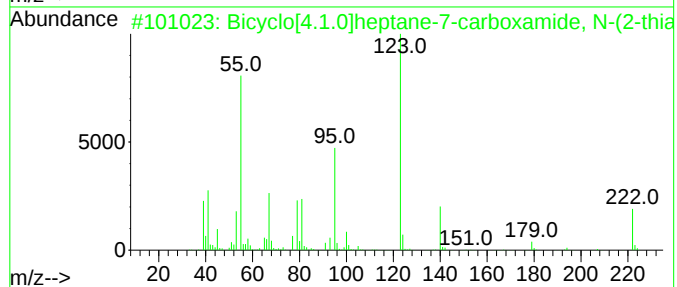
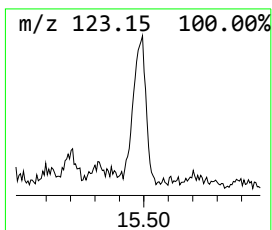
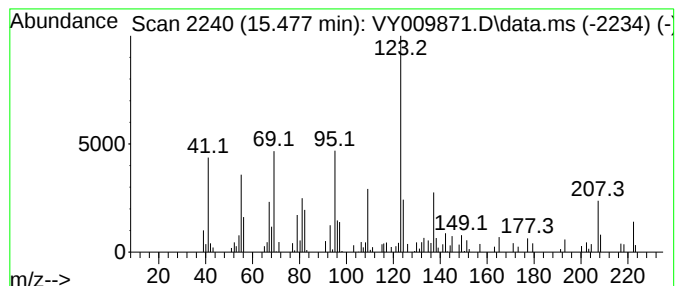
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Peak Number 6 Bicyclo[4.1.0]heptane-7-car... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.477	7.57 ug/l	59116	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.1.0]heptane-7-carboxam...	222	C11H14N2O5	329912-72-3	55
2			2,6-Naphthalenedione, octahydro-...	208	C13H20O2	057289-16-4	47
3			1-(4-Fluorophenyl)-2-(methoxymet...	222	C12H11FO3	1000388-14-4	47
4			3-(2-Ethyl-imidazol-1-yl)-propio...	168	C8H12N2O2	1010277-78-0	38
5			4-Fluorobenzoic acid, dodec-9-yn...	304	C19H25FO2	1000282-99-8	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexane	5.728	12.4	ug/l	22893	1	7.783	92246	50.0
Decahydro-1,1,4...	12.093	15.9	ug/l	71270	3	11.489	224739	50.0
unknown13.184	13.184	6.2	ug/l	48081	4	13.422	390219	50.0
Bicyclo[4.1.0]h...	15.477	7.6	ug/l	59116	4	13.422	390219	50.0