

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060321\
 Data File : VY004938.D
 Acq On : 03 Jun 2021 15:49
 Operator : SY/MD
 Sample : M2589-08
 Misc : 6.27G/5ML/MSVOA_Y/SOIL
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 18-B9(2-4)

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\82Y060221S.M
 Title : SW846 8260

Signal : TIC: VY004938.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.869	6	8	28	rVB2	52967	129305	6.91%	1.311%
2	2.253	63	71	78	rVB2	17772	39852	2.13%	0.404%
3	3.259	230	236	246	rVB4	9236	21877	1.17%	0.222%
4	4.204	383	391	401	rBV	9339	23922	1.28%	0.243%
5	4.728	464	477	484	rBV4	8602	31551	1.69%	0.320%
6	7.728	958	969	974	rBV2	157277	362785	19.38%	3.678%
7	7.795	974	980	991	rVB	263281	610468	32.61%	6.189%
8	8.155	1028	1039	1050	rBV2	202438	491757	26.27%	4.985%
9	8.697	1119	1128	1142	rVB	469262	899396	48.04%	9.118%
10	9.185	1202	1208	1215	rVB4	9448	20230	1.08%	0.205%
11	10.185	1364	1372	1378	rBV	739336	1242498	66.37%	12.596%
12	10.246	1378	1382	1389	rVB	34205	58078	3.10%	0.589%
13	11.496	1578	1587	1596	rBV	704231	1134283	60.59%	11.499%
14	11.593	1596	1603	1607	rBV3	13223	24507	1.31%	0.248%
15	11.703	1612	1621	1640	rVB	38224	95736	5.11%	0.971%
16	12.032	1661	1675	1683	rBV5	23374	64061	3.42%	0.649%
17	12.337	1717	1725	1733	rVV	276028	436330	23.31%	4.424%
18	12.489	1742	1750	1757	rBV2	1046324	1872053	100.00%	18.979%
19	12.550	1757	1760	1762	rVV3	18529	26328	1.41%	0.267%
20	12.587	1762	1766	1771	rVV	29658	49118	2.62%	0.498%
21	12.648	1771	1776	1784	rVB4	12023	26556	1.42%	0.269%
22	12.733	1784	1790	1794	rBV	16757	28772	1.54%	0.292%
23	12.812	1798	1803	1810	rVV2	35012	58882	3.15%	0.597%
24	12.898	1810	1817	1823	rVV	43024	73913	3.95%	0.749%
25	12.977	1823	1830	1837	rVB	13733	28184	1.51%	0.286%
26	13.123	1849	1854	1859	rBV	37683	59935	3.20%	0.608%
27	13.343	1884	1890	1892	rVV4	18946	37651	2.01%	0.382%
28	13.373	1892	1895	1898	rVV	25633	38951	2.08%	0.395%
29	13.428	1898	1904	1919	rVB	594651	962493	51.41%	9.758%
30	13.629	1932	1937	1940	rBV2	18294	28424	1.52%	0.288%
31	13.666	1940	1943	1951	rVB2	13907	24451	1.31%	0.248%
32	13.965	1987	1992	1999	rVB2	35062	60627	3.24%	0.615%
33	14.080	2006	2011	2015	rBV2	15827	25074	1.34%	0.254%
34	14.684	2103	2110	2115	rBV3	22885	50690	2.71%	0.514%
35	15.239	2192	2201	2209	rBV	236758	403215	21.54%	4.088%
36	16.293	2367	2374	2382	rVV	81355	157039	8.39%	1.592%

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18-B9(2-4)

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

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37	16.495	2399	2407	2414	rBV	78270	164865	8.81%	1.671%
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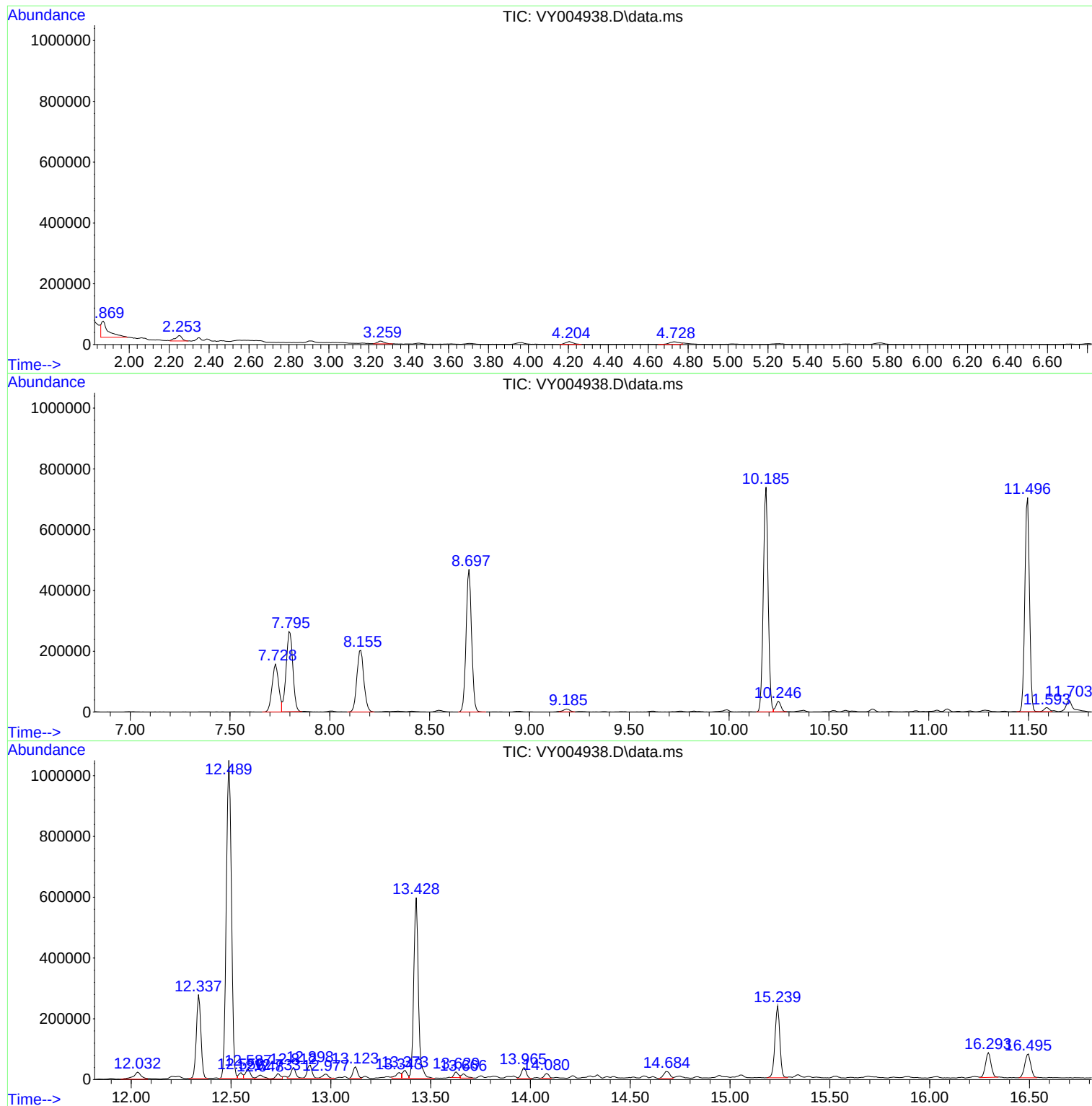
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060221S.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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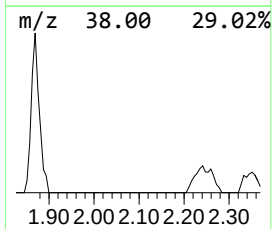
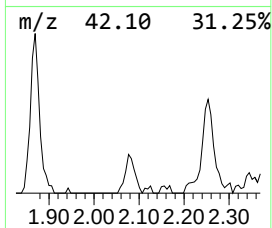
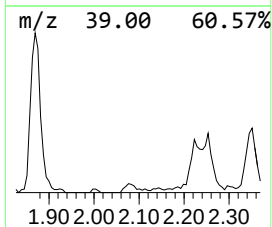
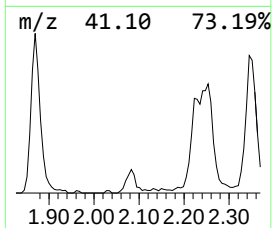
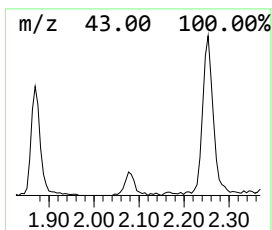
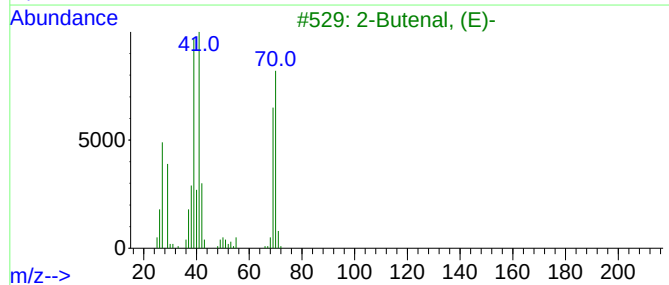
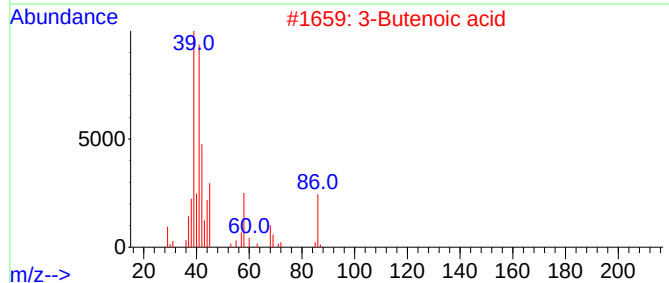
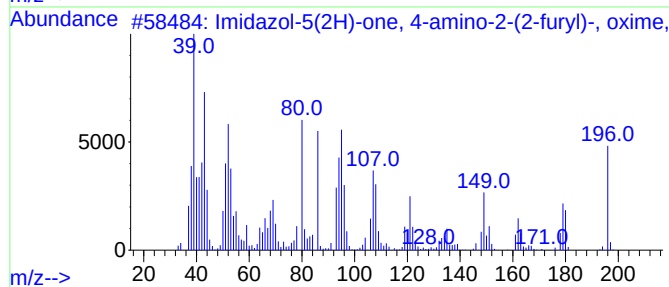
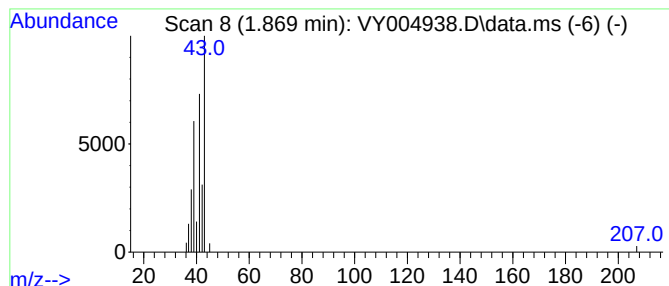
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060221S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Imidazol-5(2H)-one, 4-amino... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.869	10.59 ug/l	129305	Pentafluorobenzene	7.801

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Imidazol-5(2H)-one, 4-amino-2-(2...	196	C7H8N4O3	318259-17-5	50
2			3-Butenoic acid	86	C4H6O2	000625-38-7	47
3			2-Butenal, (E)-	70	C4H6O	000123-73-9	25
4			2-Hexenal, (E)-	98	C6H10O	006728-26-3	9
5			2H-Pyrano[3,2-b]pyridine	133	C8H7NO	004767-91-3	9



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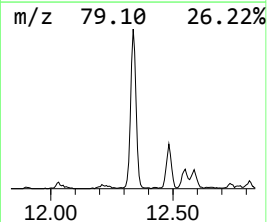
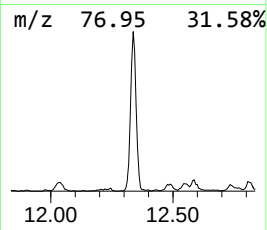
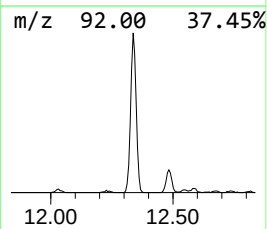
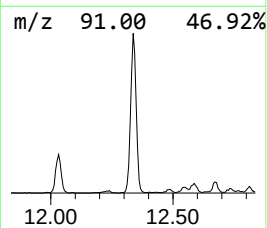
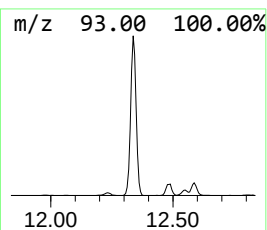
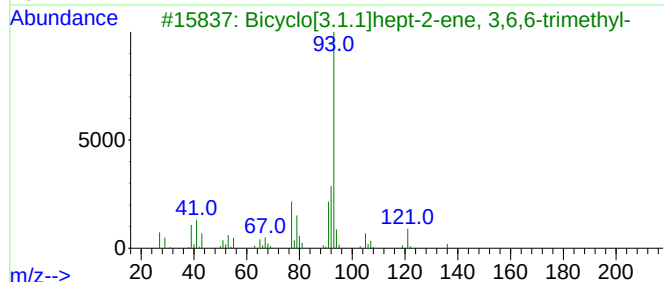
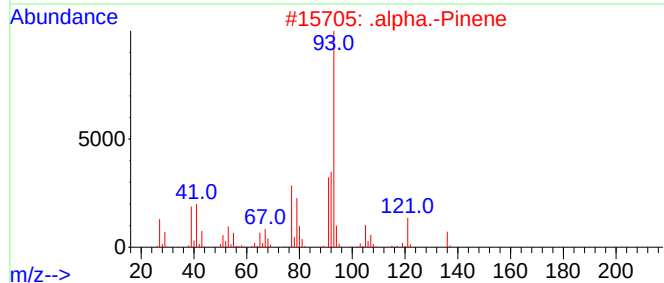
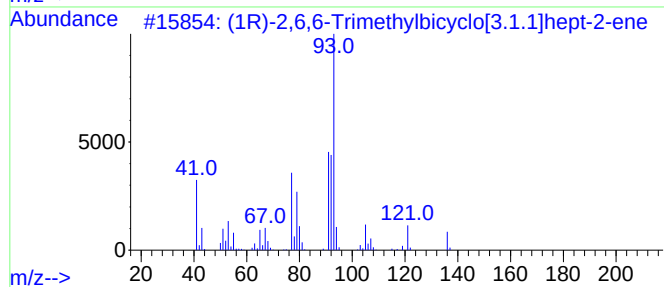
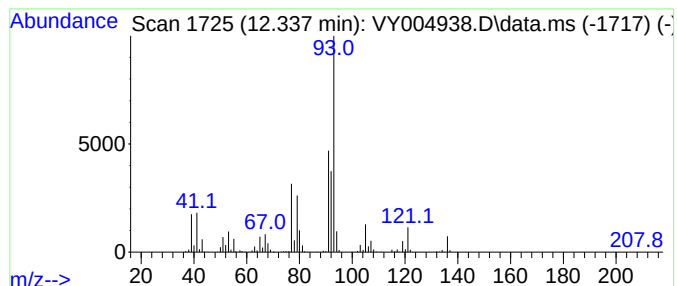
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TIC Integration Parameters: LSCINT.P

Peak Number 2 (1R)-2,6,6-Trimethylbicyclo... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.337	19.23 ug/l	436330	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	97		
2	.alpha.-Pinene	136	C10H16	000080-56-8	97		
3	Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	136	C10H16	004889-83-2	91		
4	(+)-3-Carene	136	C10H16	000498-15-7	91		
5	(1S)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-26-4	90		



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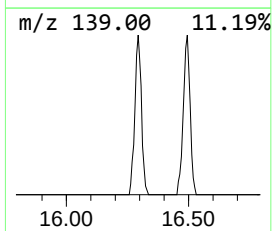
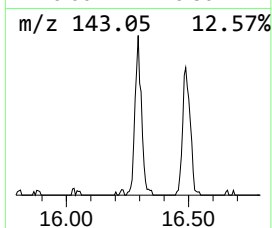
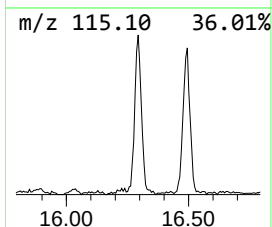
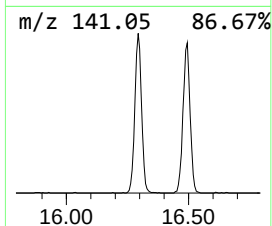
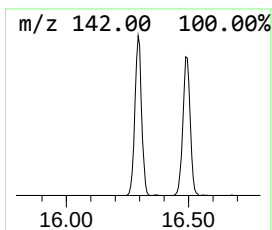
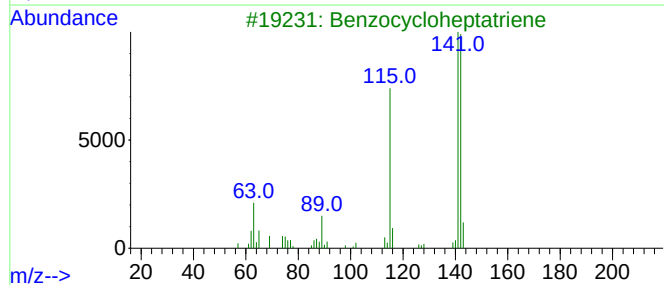
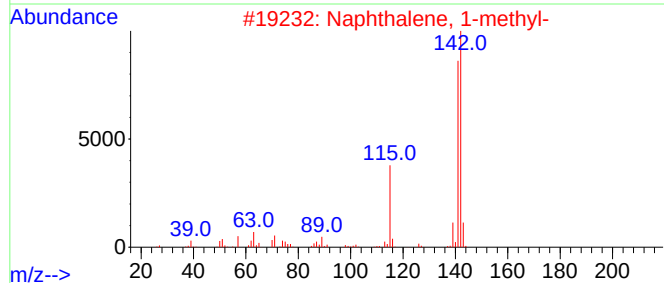
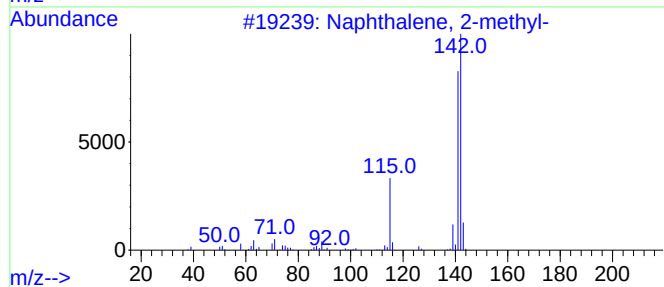
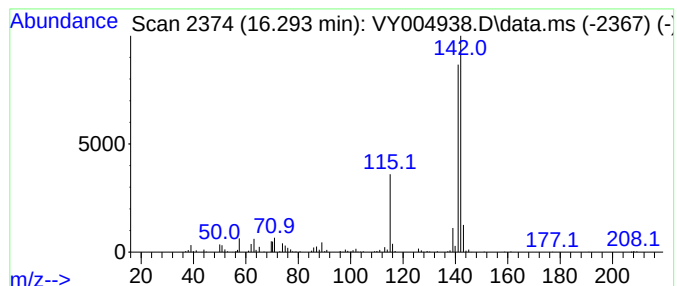
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Naphthalene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.294	8.16 ug/l	157039	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	90
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	87
5			Spiro(tricyclo[6.2.1.0(2,7)]unde...	186	C13H14O	1000210-02-3	78



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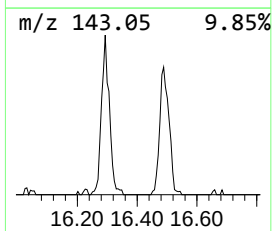
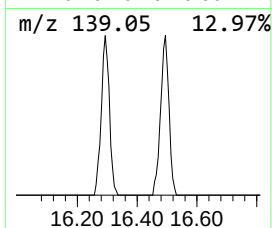
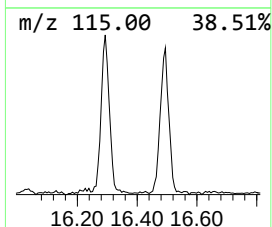
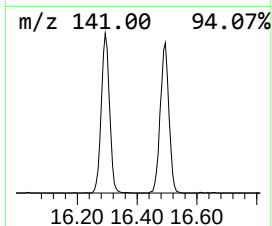
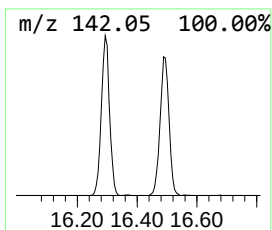
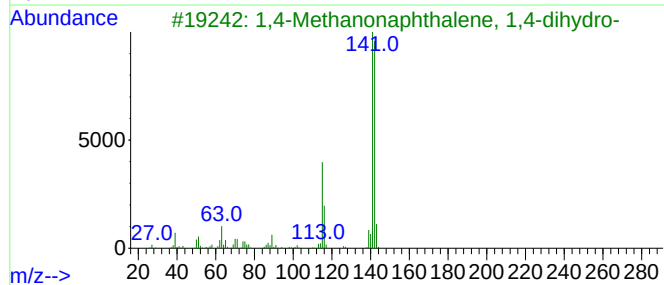
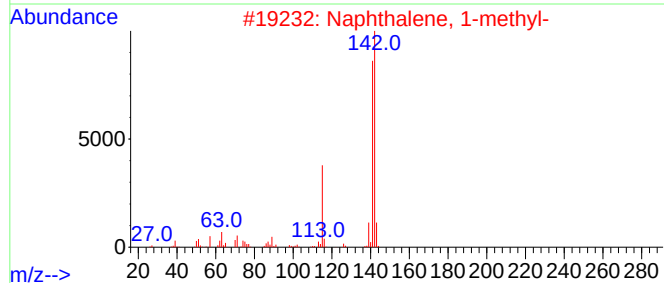
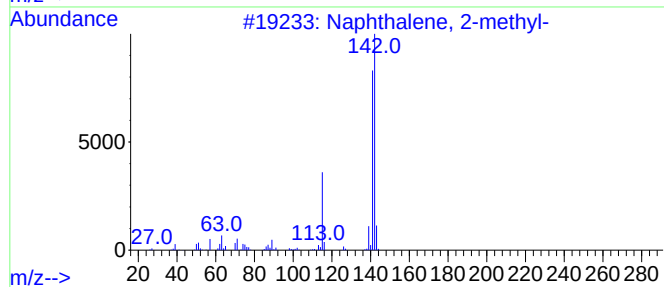
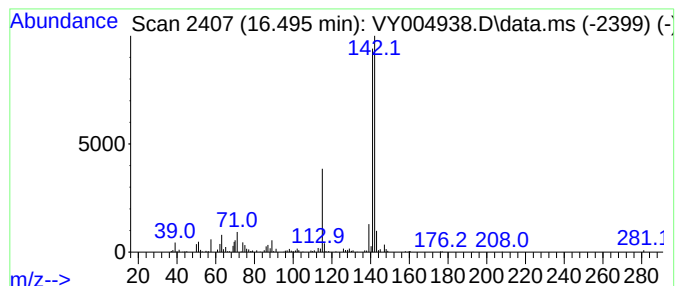
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1,4-Methanonaphthalene, 1,4... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.495	8.56 ug/l	164865	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4			Benzocycloheptatriene	142	C11H10	000264-09-5	90
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Imidazol-5(2H)-...	1.869	10.6	ug/l	129305	1	7.801	610468	50.0
(1R)-2,6,6-Trim...	12.337	19.2	ug/l	436330	3	11.496	1134280	50.0
Naphthalene, 1-...	16.294	8.2	ug/l	157039	4	13.428	962493	50.0
1,4-Methanonaph...	16.495	8.6	ug/l	164865	4	13.428	962493	50.0