

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX110918\
 Data File : VX005882.D
 Acq On : 10 Nov 2018 01:18
 Operator : JC/MD
 Sample : J5889-05
 Misc : 14.24g/5mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 WALL-E

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.672	63	85	86	rBV5	13363	56962	10.34%	1.521%
2	2.806	258	271	276	rBV3	3028	8585	1.56%	0.229%
3	3.019	302	306	316	rVB2	2636	6177	1.12%	0.165%
4	5.507	698	714	727	rBV3	65970	198641	36.05%	5.304%
5	5.653	727	738	758	rVB2	130258	368233	66.82%	9.833%
6	6.068	793	806	820	rBV	80082	210058	38.12%	5.609%
7	6.860	925	936	950	rBV	175299	431206	78.25%	11.514%
8	8.713	1233	1240	1249	rBV	346704	551058	100.00%	14.714%
9	10.116	1464	1470	1486	rBV	338599	483458	87.73%	12.909%
10	11.140	1632	1638	1649	rBV	304860	394471	71.58%	10.533%
11	11.670	1711	1725	1726	rBV8	2091	6290	1.14%	0.168%
12	11.810	1744	1748	1751	rBV2	3623	5534	1.00%	0.148%
13	12.079	1787	1792	1800	rBV	420416	523676	95.03%	13.983%
14	12.896	1920	1926	1928	rBV4	4415	8680	1.58%	0.232%
15	13.481	2019	2022	2031	rVB6	7484	19021	3.45%	0.508%
16	13.603	2033	2042	2052	rVB6	9678	33325	6.05%	0.890%
17	13.902	2087	2091	2099	rVB7	10232	21099	3.83%	0.563%
18	13.987	2102	2105	2114	rVB8	5202	12510	2.27%	0.334%
19	14.097	2119	2123	2125	rBV4	3835	5757	1.04%	0.154%
20	14.133	2125	2129	2132	rBV3	6662	11732	2.13%	0.313%
21	14.273	2147	2152	2160	rVB6	20074	52994	9.62%	1.415%
22	14.377	2163	2169	2175	rBV2	13383	30585	5.55%	0.817%
23	14.542	2192	2196	2200	rBV6	5011	9938	1.80%	0.265%
24	14.676	2214	2218	2220	rBV4	10201	16419	2.98%	0.438%
25	14.694	2220	2221	2225	rVB	12777	11381	2.07%	0.304%
26	14.792	2230	2237	2243	rBV3	21088	53442	9.70%	1.427%
27	15.066	2276	2282	2289	rVB2	14989	33375	6.06%	0.891%
28	15.255	2305	2313	2315	rBV5	8825	20286	3.68%	0.542%
29	15.353	2324	2329	2332	rBV7	6398	12046	2.19%	0.322%
30	15.456	2341	2346	2347	rBV4	4982	7692	1.40%	0.205%
31	15.554	2356	2362	2371	rVB6	21762	49925	9.06%	1.333%
32	15.688	2381	2384	2387	rVV2	7467	11627	2.11%	0.310%
33	15.731	2388	2391	2399	rVB5	15199	31208	5.66%	0.833%
34	16.072	2443	2447	2454	rVB8	4347	9503	1.72%	0.254%

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Title : SW846 8260

35	16.163	2460	2462	2472	rVB7	4001	6958	1.26%	0.186%
36	16.450	2504	2509	2516	rVB6	3450	6357	1.15%	0.170%
37	16.694	2538	2549	2555	rBV5	5620	16246	2.95%	0.434%
38	16.755	2555	2559	2564	rBV3	4494	8566	1.55%	0.229%

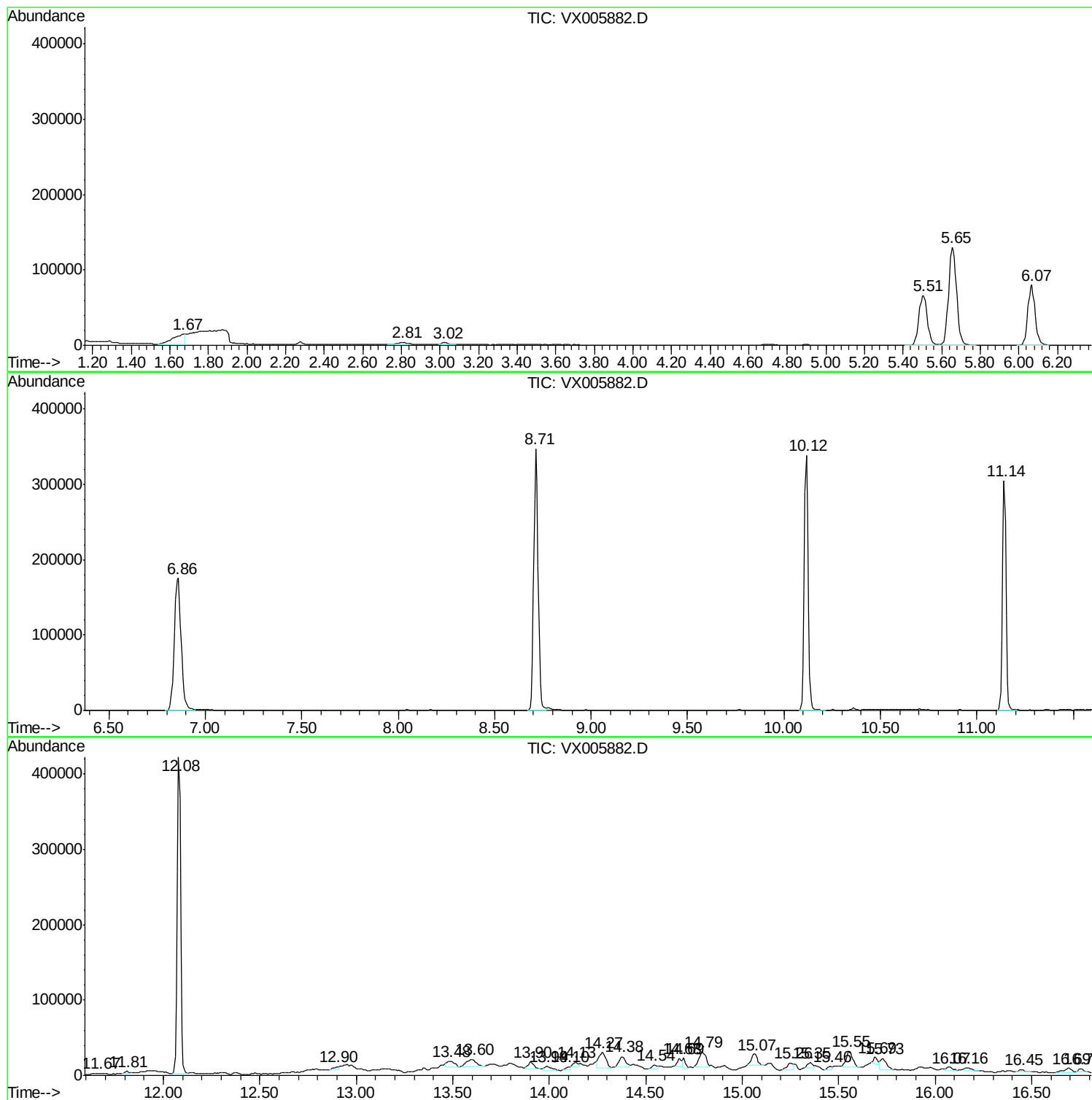
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Quant Title : SW846 8260

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



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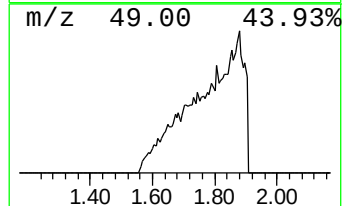
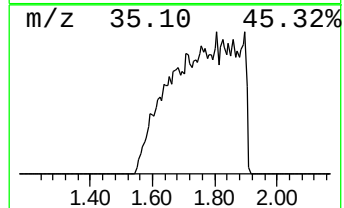
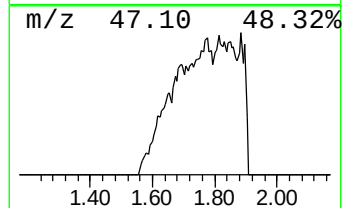
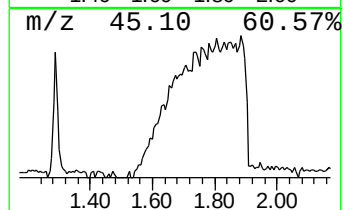
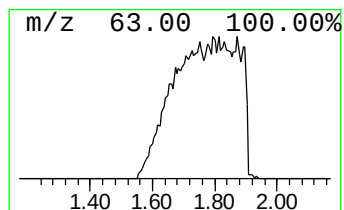
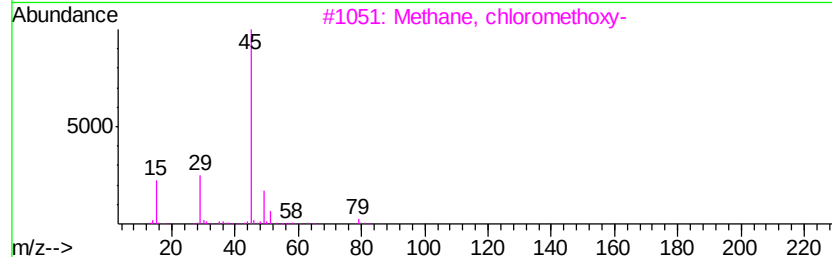
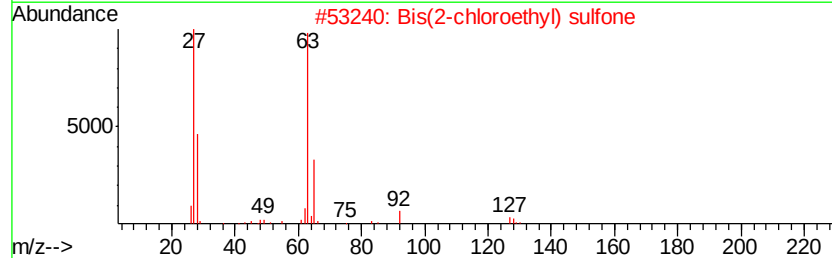
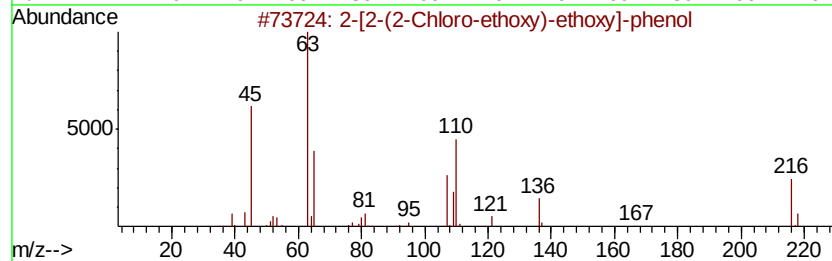
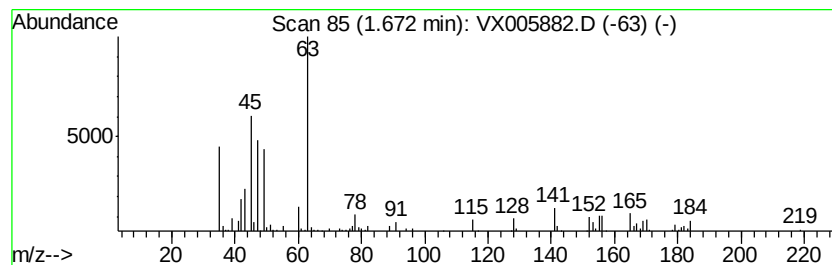
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown1.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.67	7.73 ug/l	56962	Pentafluorobenzene	5.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-[2-(2-Chloro-ethoxy)-ethoxy]-p...	216	C10H13ClO3	1000317-46-1	28
2			Bis(2-chloroethyl) sulfone	190	C4H8Cl2O2S	000471-03-4	12
3			Methane, chloromethoxy-	80	C2H5ClO	000107-30-2	9
4			1-Bromo-1-chloroethane	142	C2H4BrCl	000593-96-4	9
5			Carbonfluoridodithioic acid, tri...	164	C2F4S2	000371-73-3	9



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ALS Vial : 33 Sample Multiplier: 1

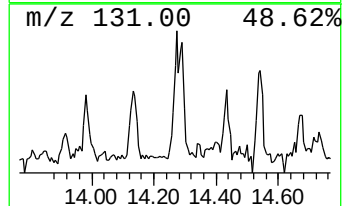
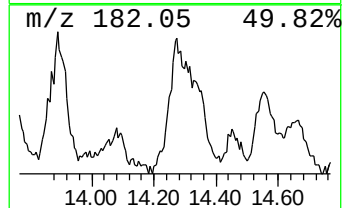
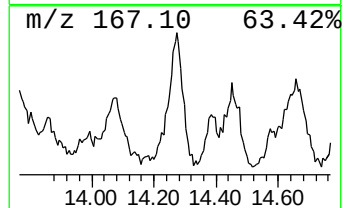
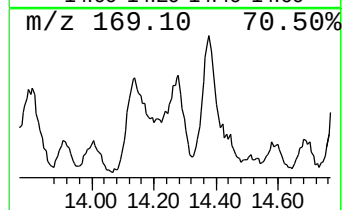
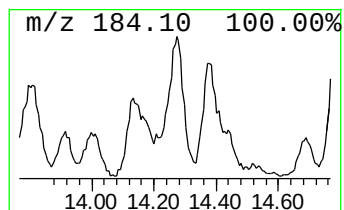
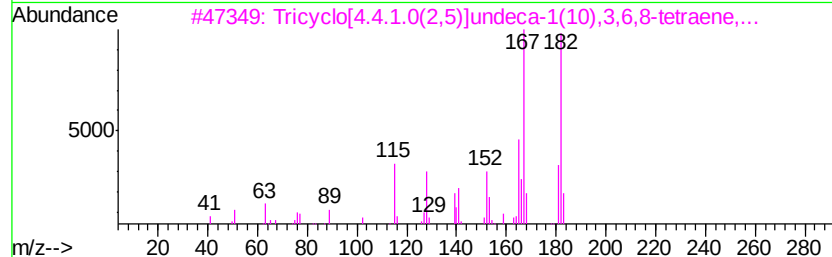
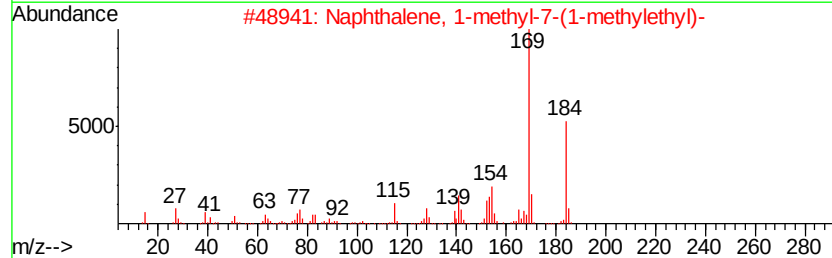
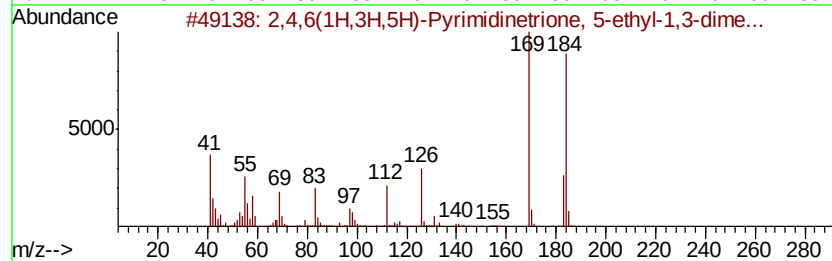
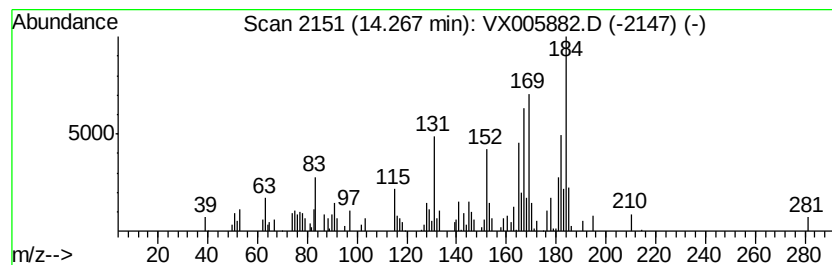
Instrument :
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Peak Number 2 unknown14.27 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.27	5.06 ug/l	52994	1,4-Dichlorobenzene-d4	12.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,6(1H,3H,5H)-Pyrimidinetrione...	184	C8H12N2O3	007391-61-9	43
2	Naphthalene, 1-methyl-7-(1-methy...	184	C14H16	000490-65-3	41
3	Tricyclo[4.4.1.0(2,5)]undeca-1(1...	182	C14H14	055836-29-8	38
4	1,1'-Biphenyl, 4-methoxy-	184	C13H12O	000613-37-6	38
5	1,1'-Biphenyl, 2-ethyl-	182	C14H14	001812-51-7	35



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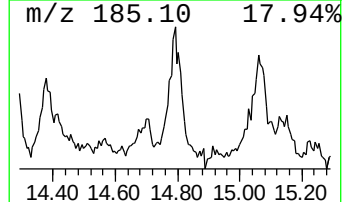
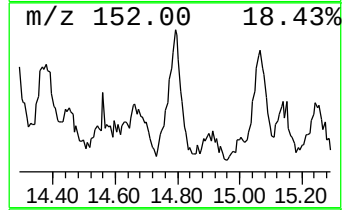
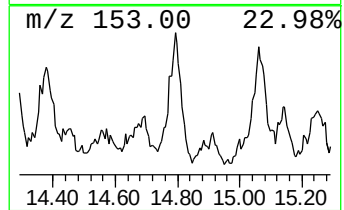
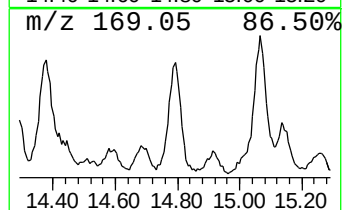
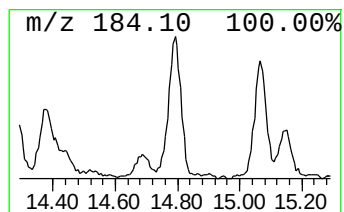
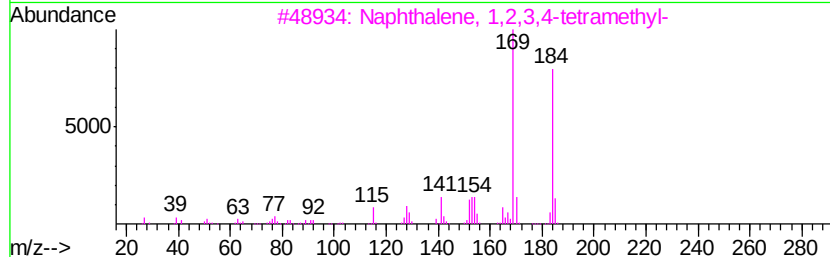
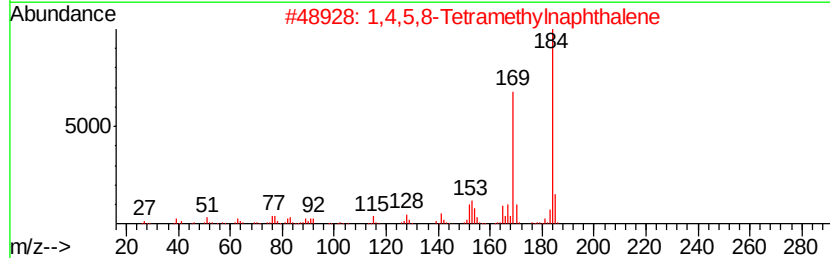
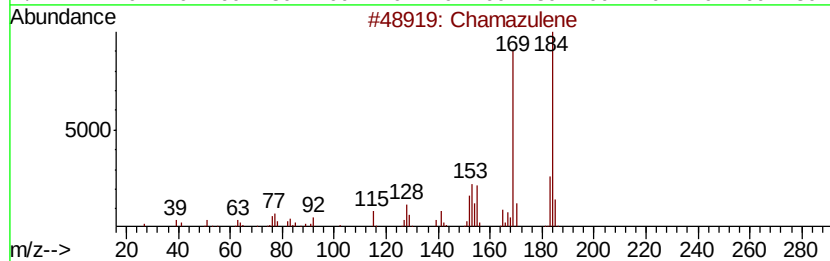
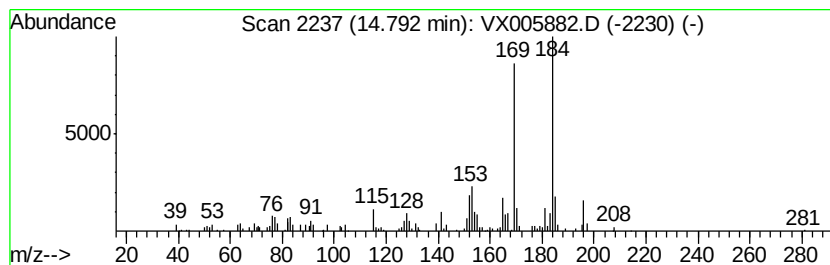
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Chamazulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	5.10 ug/l	53442	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Chamazulene	184 C14H16	000529-05-5	91
2	1,4,5,8-Tetramethylnaphthalene	184 C14H16	002717-39-7	91
3	Naphthalene, 1,2,3,4-tetramethyl-	184 C14H16	003031-15-0	81
4	Cyclopentene, 1,2-dimethyl-4-met...	184 C14H16	1000152-22-4	81
5	1,1'-Biphenyl, 2-methoxy-	184 C13H12O	000086-26-0	74



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.67	1.67	7.7	ug/l	56962	1	5.65	368233	50.0
unknown14.27	14.27	5.1	ug/l	52994	4	12.08	523676	50.0
Chamazulene	14.79	5.1	ug/l	53442	4	12.08	523676	50.0