

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
 Data File : VX028211.D
 Acq On : 20 Apr 2022 20:27
 Operator : JC/MD
 Sample : N2459-08
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 31578

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_X\Method\82X041922W.M
 Title : SW846 8260

Signal : TIC: VX028211.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	33	rBV3	15073	34572	1.43%	0.205%
2	1.374	42	47	52	rVB	22142	25173	1.04%	0.149%
3	1.556	69	77	83	rBV6	15207	30463	1.26%	0.180%
4	1.752	104	109	117	rBV	31614	44647	1.85%	0.264%
5	5.391	691	706	720	rBV	300980	879338	36.39%	5.206%
6	5.556	722	733	754	rVB	409039	1176527	48.69%	6.966%
7	5.958	788	799	807	rBV	295248	787166	32.58%	4.661%
8	6.043	807	813	826	rVB2	63023	171885	7.11%	1.018%
9	6.763	921	931	949	rBV	644843	1530813	63.35%	9.063%
10	8.653	1233	1241	1247	rBV	1548923	2416316	100.00%	14.306%
11	8.720	1247	1252	1262	rVB	238152	371943	15.39%	2.202%
12	10.055	1465	1471	1481	rBV	1429577	1887550	78.12%	11.175%
13	10.195	1489	1494	1506	rVB	61398	82935	3.43%	0.491%
14	10.640	1562	1567	1579	rBV	233766	305292	12.63%	1.808%
15	11.085	1634	1640	1652	rBV	1295636	1702039	70.44%	10.077%
16	11.402	1684	1692	1696	rBV	34947	51334	2.12%	0.304%
17	11.451	1696	1700	1709	rVB	67223	84016	3.48%	0.497%
18	11.616	1719	1727	1734	rBV	66069	86530	3.58%	0.512%
19	11.969	1780	1785	1788	rBV	21054	26839	1.11%	0.159%
20	12.024	1788	1794	1800	rVV	1481771	1861185	77.03%	11.019%
21	12.085	1800	1804	1810	rVB	130957	163715	6.78%	0.969%
22	12.244	1824	1830	1834	rBV2	87661	129753	5.37%	0.768%
23	12.317	1838	1842	1848	rVV2	73391	98330	4.07%	0.582%
24	12.463	1862	1866	1871	rVB	40836	48543	2.01%	0.287%
25	12.615	1886	1891	1894	rBV	61392	75620	3.13%	0.448%
26	12.701	1900	1905	1914	rBV2	60386	114027	4.72%	0.675%
27	12.847	1924	1929	1934	rVB2	38076	52885	2.19%	0.313%
28	12.920	1934	1941	1945	rBV	44806	59927	2.48%	0.355%
29	12.963	1945	1948	1954	rVB	69509	83477	3.45%	0.494%
30	13.042	1954	1961	1964	rBV2	18777	42748	1.77%	0.253%
31	13.170	1979	1982	1985	rVB	30548	35128	1.45%	0.208%
32	13.256	1992	1996	1998	rBV2	18520	28112	1.16%	0.166%
33	13.292	1998	2002	2007	rVB2	208540	279344	11.56%	1.654%
34	13.420	2018	2023	2033	rVB	158591	209380	8.67%	1.240%
35	13.506	2033	2037	2040	rBV3	19411	27162	1.12%	0.161%
36	13.542	2040	2043	2046	rBV	27241	35723	1.48%	0.212%

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37	13.585	2046	2050	2055	rVV3	50234	78589	3.25%	0.465%
38	13.664	2060	2063	2069	rVB2	61650	91250	3.78%	0.540%
39	13.780	2079	2082	2089	rVB2	16794	36738	1.52%	0.218%
40	13.853	2089	2094	2100	rVB	72836	97389	4.03%	0.577%
41	13.926	2100	2106	2110	rBV2	88449	123625	5.12%	0.732%
42	13.969	2110	2113	2117	rVB	23619	30031	1.24%	0.178%
43	14.079	2126	2131	2135	rBV	44294	61020	2.53%	0.361%
44	14.231	2148	2156	2162	rBV	154186	272293	11.27%	1.612%
45	14.322	2167	2171	2175	rVV	28780	37824	1.57%	0.224%
46	14.371	2175	2179	2184	rVB	68146	85905	3.56%	0.509%
47	14.481	2192	2197	2202	rBV2	167601	216798	8.97%	1.284%
48	14.615	2211	2219	2225	rBV3	73561	148075	6.13%	0.877%
49	14.676	2225	2229	2233	rVB	45608	64069	2.65%	0.379%
50	14.822	2249	2253	2255	rBV	29465	41199	1.71%	0.244%
51	14.847	2255	2257	2261	rVB2	32408	35446	1.47%	0.210%
52	14.902	2261	2266	2274	rBV4	36064	73107	3.03%	0.433%
53	15.054	2283	2291	2295	rBV2	19157	30016	1.24%	0.178%
54	15.182	2304	2312	2320	rBV	73256	134875	5.58%	0.799%
55	15.377	2339	2344	2352	rVB8	17722	35750	1.48%	0.212%
56	15.481	2352	2361	2364	rBV4	28670	48928	2.02%	0.290%
57	15.523	2365	2368	2373	rVB3	16735	26739	1.11%	0.158%
58	15.615	2378	2383	2386	rVV3	28842	50584	2.09%	0.299%
59	15.652	2386	2389	2397	rVB5	15584	29419	1.22%	0.174%

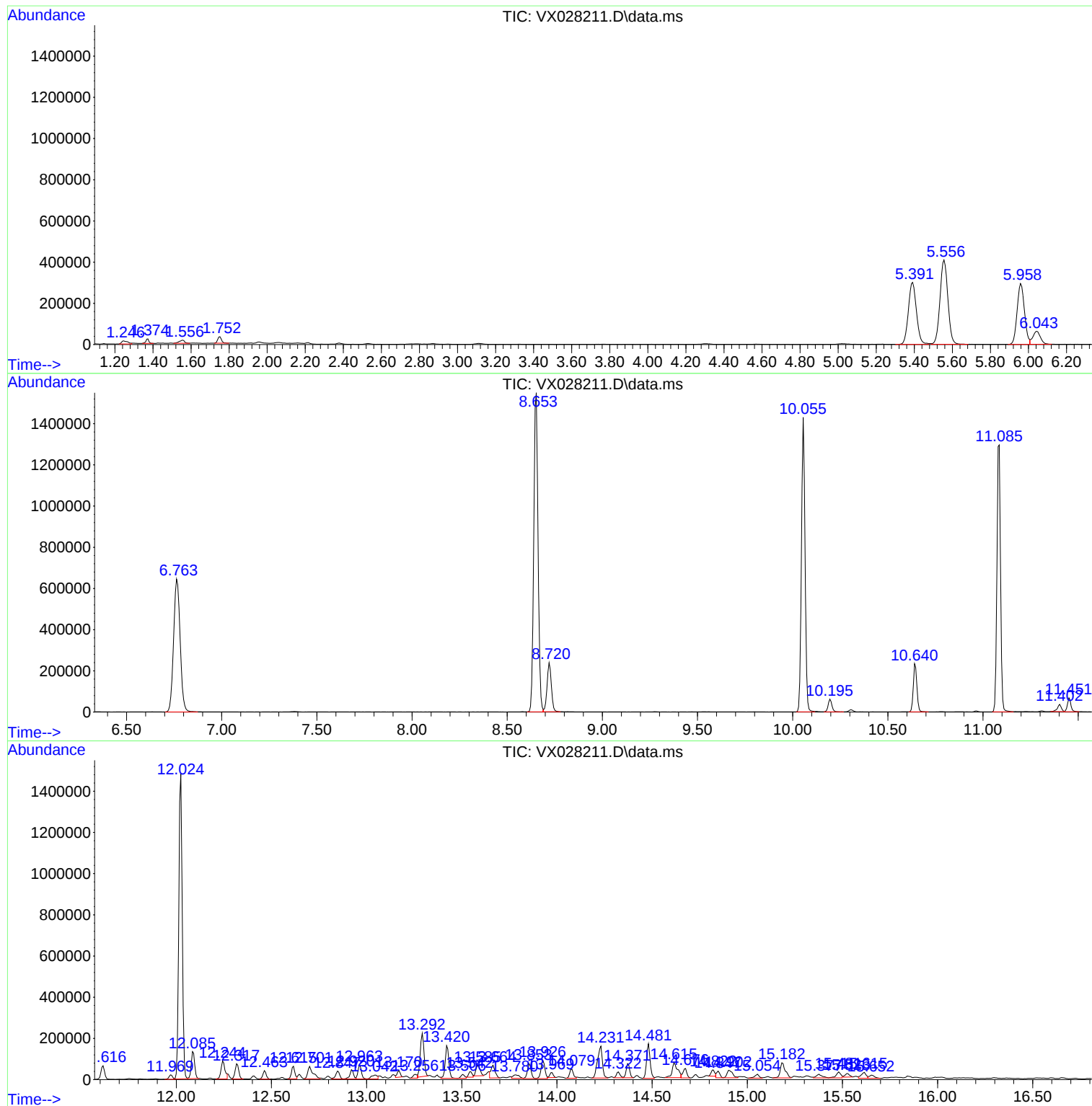
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Quant Title : SW846 8260

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



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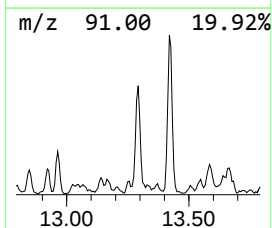
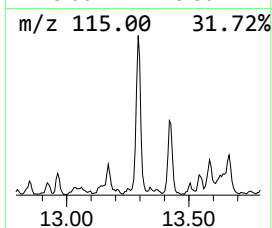
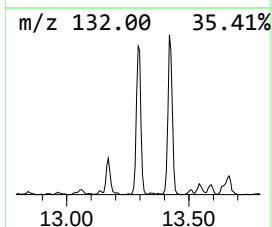
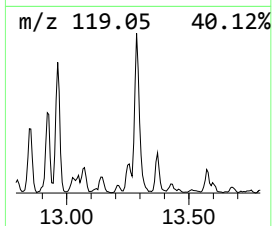
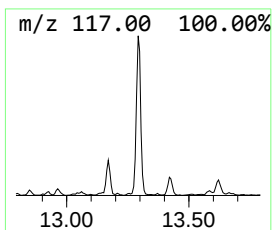
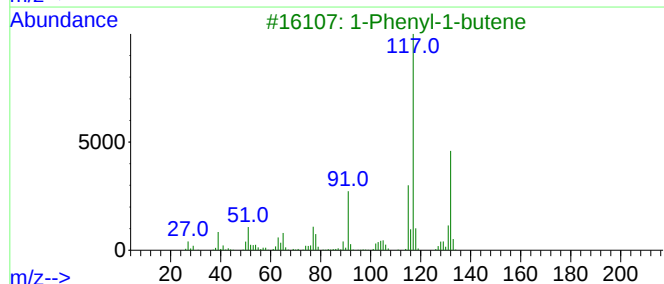
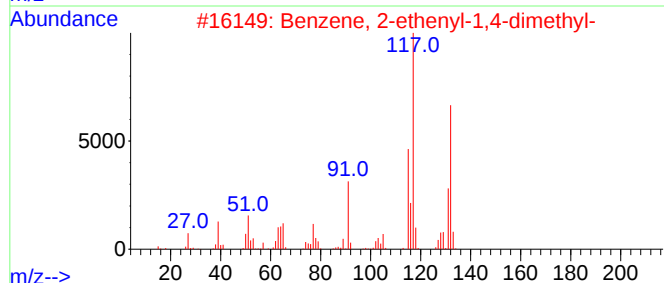
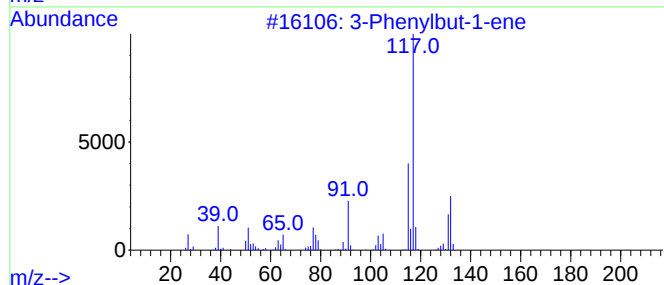
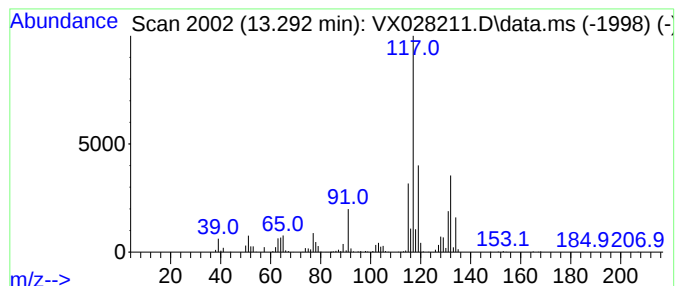
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 1 3-Phenylbut-1-ene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	7.50 ug/l	279344	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
2		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	70
3		1-Phenyl-1-butene	132	C10H12	000824-90-8	70
4		Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	70
5		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	70



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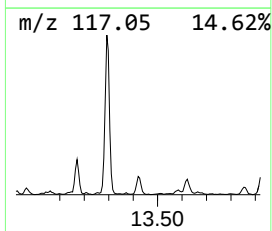
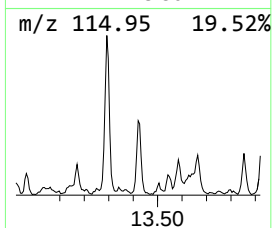
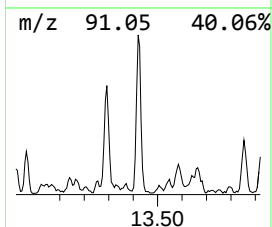
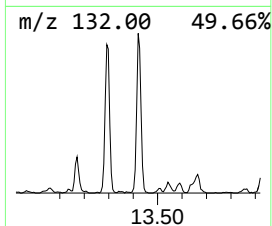
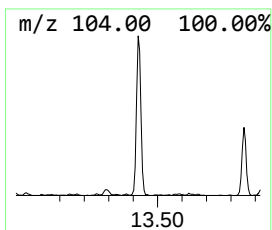
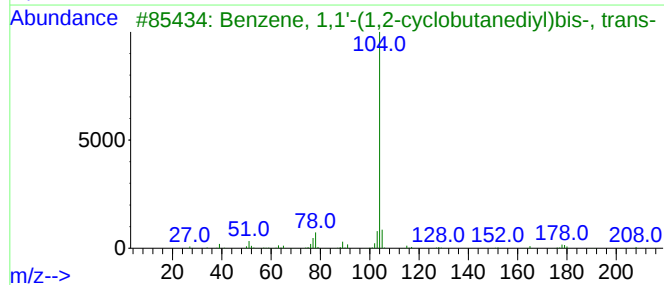
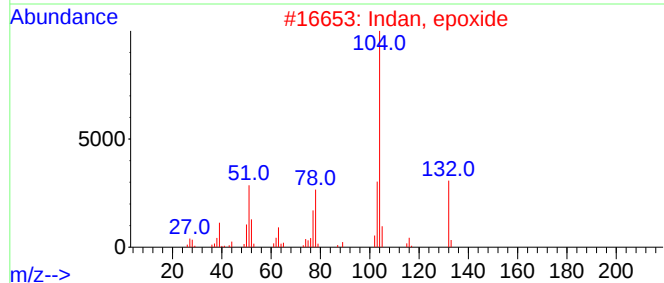
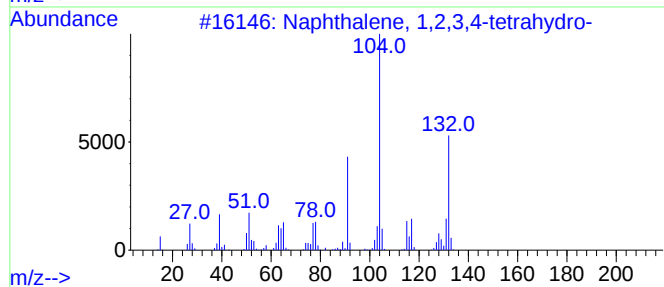
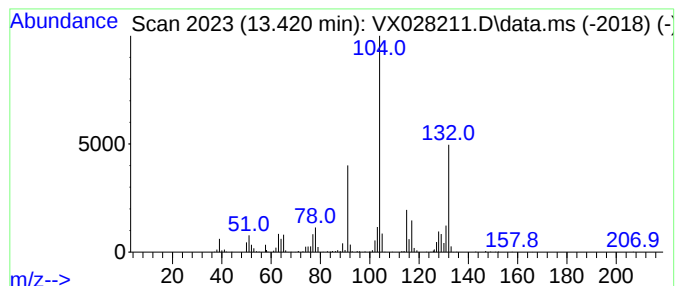
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	5.62 ug/l	209380	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	91
2			Indan, epoxide	132	C9H8O	000768-22-9	60
3			Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	020071-09-4	35
4			Styrene	104	C8H8	000100-42-5	27
5			Benzeneacetic acid, 2-phenylethy...	240	C16H16O2	000102-20-5	27



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Instrument :
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ClientSampleId :
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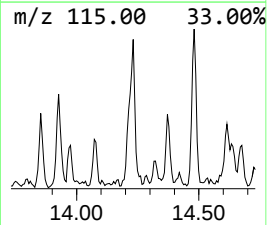
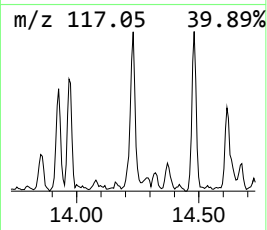
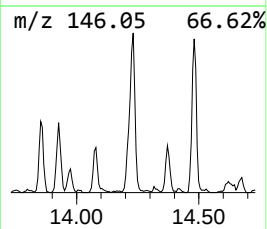
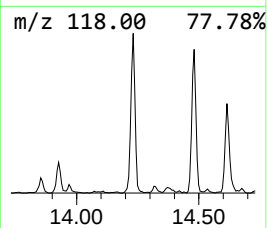
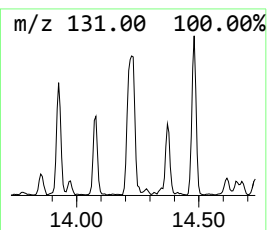
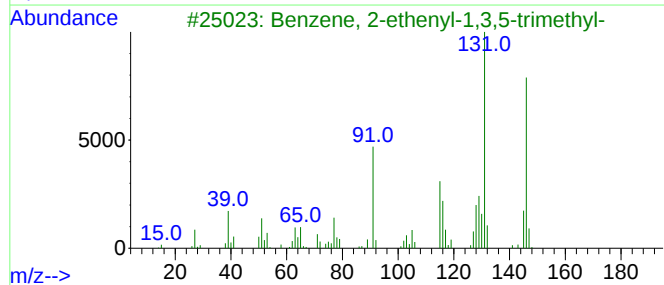
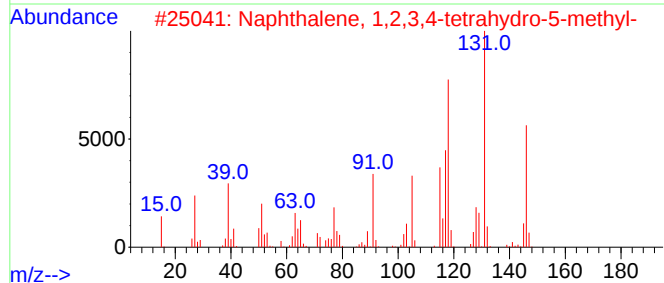
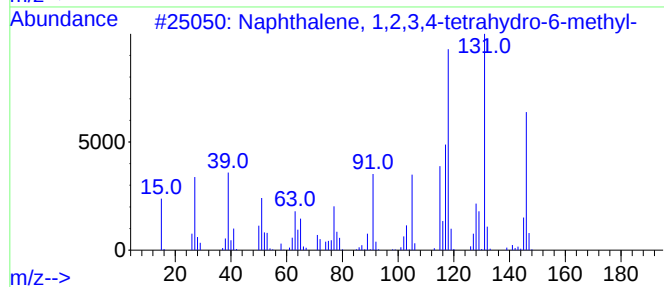
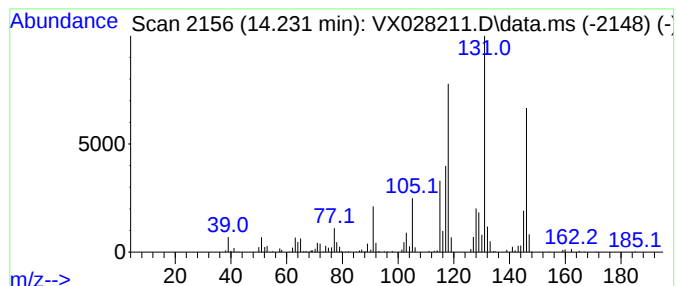
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.231	7.32 ug/l	272293	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	95
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	94
3			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	78
4			1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	62
5			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	55



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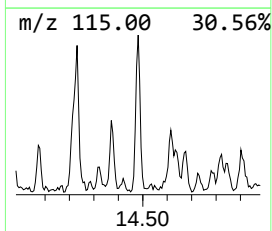
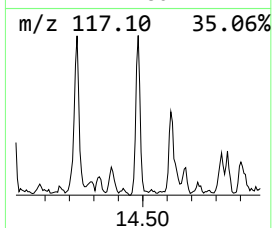
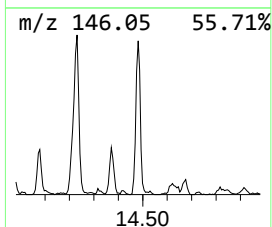
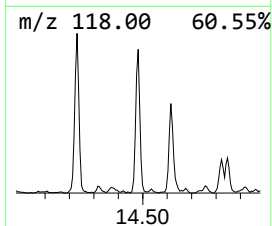
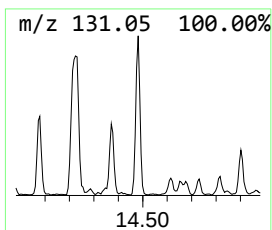
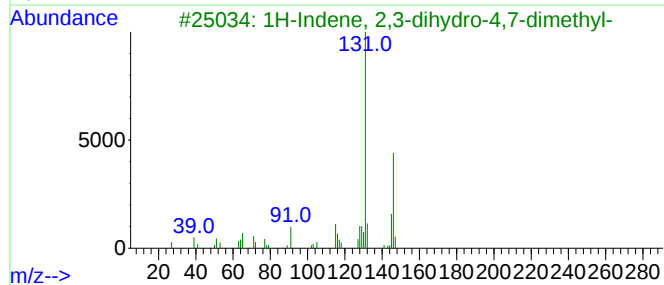
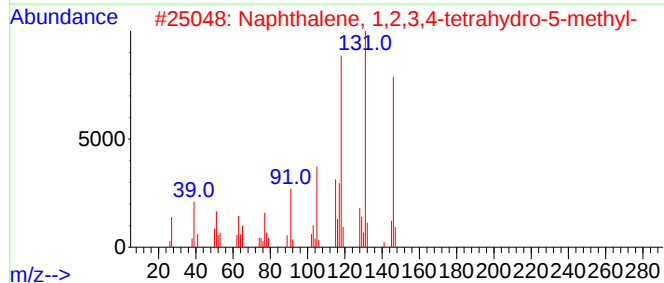
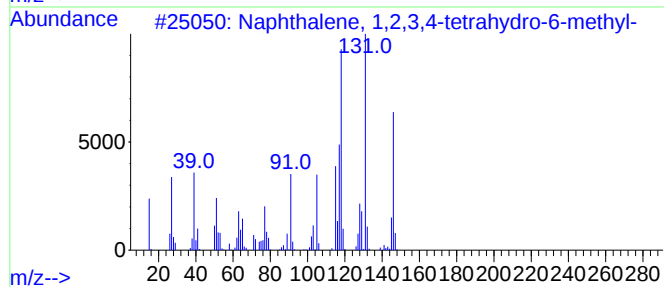
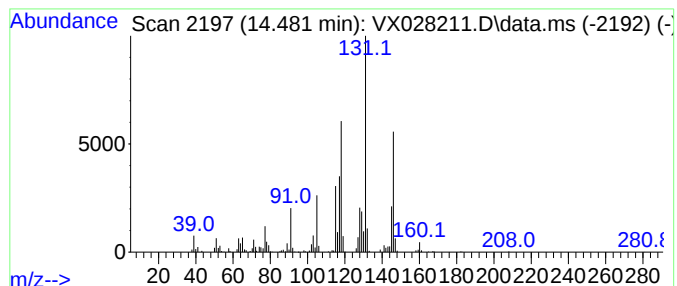
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 4 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.481	5.82 ug/l	216798	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	95
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	94
3			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	76
4			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	64
5			1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	62



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Phenylbut-1-ene	13.292	7.5	ug/l	279344	4	12.024	1861190	50.0
Naphthalene, 1,...	13.420	5.6	ug/l	209380	4	12.024	1861190	50.0
Naphthalene, 1,...	14.231	7.3	ug/l	272293	4	12.024	1861190	50.0
Naphthalene, 1,...	14.481	5.8	ug/l	216798	4	12.024	1861190	50.0