

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082923\
 Data File : VX037350.D
 Acq On : 29 Aug 2023 18:30
 Operator : JC/MD
 Sample : 04110-14
 Misc : 4.78g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 TP-21(3-4)

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_X\Method\82X081723W.M
 Title : SW846 8260

Signal : TIC: VX037350.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	22	28	34	rBV3	16152	35482	5.02%	0.571%
2	1.624	84	88	97	rBV	57522	69041	9.77%	1.111%
3	1.709	98	102	109	rVB	10563	13119	1.86%	0.211%
4	1.886	127	131	138	rVB5	5207	11338	1.60%	0.182%
5	2.733	264	270	273	rBV4	5260	10992	1.56%	0.177%
6	2.782	273	278	290	rVB2	12784	31062	4.40%	0.500%
7	2.946	297	305	316	rBV	7348	17710	2.51%	0.285%
8	3.062	316	324	333	rVB3	6683	15494	2.19%	0.249%
9	3.410	374	381	389	rBV2	4148	9804	1.39%	0.158%
10	4.276	513	523	534	rVB	11690	32529	4.60%	0.523%
11	5.385	694	705	714	rBV2	73309	224590	31.79%	3.613%
12	5.544	722	731	751	rVB	146124	429170	60.74%	6.904%
13	5.812	766	775	787	rVB7	3833	11932	1.69%	0.192%
14	5.952	789	798	806	rVV	82167	216534	30.65%	3.483%
15	6.031	807	811	820	rVV	10683	26309	3.72%	0.423%
16	6.141	820	829	839	rVV5	5126	15553	2.20%	0.250%
17	6.245	839	846	853	rVV3	4611	11847	1.68%	0.191%
18	6.342	853	862	873	rVB3	8953	24695	3.50%	0.397%
19	6.592	898	903	911	rVB4	3413	7881	1.12%	0.127%
20	6.757	920	930	951	rBV	211651	502637	71.14%	8.086%
21	7.373	1021	1031	1040	rVB2	78646	178444	25.26%	2.871%
22	7.653	1071	1077	1083	rBV2	3747	7241	1.02%	0.116%
23	7.769	1090	1096	1103	rVB4	5459	11055	1.56%	0.178%
24	7.952	1120	1126	1135	rBV3	5313	10845	1.53%	0.174%
25	8.269	1174	1178	1182	rBV2	5375	8481	1.20%	0.136%
26	8.598	1226	1232	1234	rBV2	13319	22624	3.20%	0.364%
27	8.647	1234	1240	1245	rVV	437497	706530	100.00%	11.366%
28	8.714	1245	1251	1257	rVV2	90387	229921	32.54%	3.699%
29	8.763	1257	1259	1264	rVB4	5459	8579	1.21%	0.138%
30	8.842	1269	1272	1278	rVV3	5124	8724	1.23%	0.140%
31	8.909	1278	1283	1288	rVV	9464	13350	1.89%	0.215%
32	8.970	1288	1293	1299	rVB2	13000	21984	3.11%	0.354%
33	9.275	1338	1343	1348	rVB3	5210	8144	1.15%	0.131%
34	9.384	1356	1361	1365	rBV2	6420	10382	1.47%	0.167%
35	9.506	1369	1381	1385	rBV5	4411	8924	1.26%	0.144%
36	9.561	1385	1390	1395	rVV	16207	23549	3.33%	0.379%

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37	9.616	1395	1399	1403	rVV	10181	16427	2.33%	0.264%
38	9.817	1427	1432	1442	rBV3	7946	14930	2.11%	0.240%
39	10.006	1458	1463	1466	rBV3	4177	7742	1.10%	0.125%
40	10.055	1466	1471	1478	rVV	410717	556720	78.80%	8.956%
41	10.122	1478	1482	1487	rVV	4891	8678	1.23%	0.140%
42	10.195	1487	1494	1501	rVV	14857	20822	2.95%	0.335%
43	10.299	1501	1511	1517	rVV	82132	123806	17.52%	1.992%
44	10.360	1517	1521	1532	rVB3	15798	23774	3.36%	0.382%
45	10.585	1548	1558	1562	rBV6	5172	10600	1.50%	0.171%
46	10.640	1562	1567	1576	rVB	55798	77065	10.91%	1.240%
47	10.756	1581	1586	1587	rBV	6746	9041	1.28%	0.145%
48	10.780	1587	1590	1595	rVB2	15085	18960	2.68%	0.305%
49	10.854	1595	1602	1606	rBV4	11919	19440	2.75%	0.313%
50	10.896	1606	1609	1615	rVB	7667	10392	1.47%	0.167%
51	10.963	1615	1620	1624	rBV	10900	14190	2.01%	0.228%
52	11.085	1634	1640	1652	rVB	314352	429658	60.81%	6.912%
53	11.219	1659	1662	1671	rVB4	5456	8709	1.23%	0.140%
54	11.305	1671	1676	1679	rBV	10084	14151	2.00%	0.228%
55	11.384	1684	1689	1695	rVV	21229	37420	5.30%	0.602%
56	11.451	1695	1700	1702	rVV	14970	22617	3.20%	0.364%
57	11.475	1702	1704	1710	rVB	19992	22345	3.16%	0.359%
58	11.616	1722	1727	1734	rBV	16834	22750	3.22%	0.366%
59	11.713	1740	1743	1746	rBV	13097	15186	2.15%	0.244%
60	11.750	1746	1749	1760	rVB	54710	76916	10.89%	1.237%
61	11.866	1760	1768	1769	rBV4	3714	7338	1.04%	0.118%
62	11.890	1769	1772	1776	rVV	8456	11276	1.60%	0.181%
63	11.945	1776	1781	1783	rVV4	6426	10143	1.44%	0.163%
64	11.969	1783	1785	1789	rVV2	9066	11036	1.56%	0.178%
65	12.024	1789	1794	1800	rVV	426220	535049	75.73%	8.607%
66	12.091	1800	1805	1813	rVV	23288	37811	5.35%	0.608%
67	12.170	1813	1818	1826	rVB8	3382	7517	1.06%	0.121%
68	12.244	1826	1830	1832	rBV2	6123	8370	1.18%	0.135%
69	12.323	1837	1843	1851	rVB4	12091	26524	3.75%	0.427%
70	12.420	1851	1859	1864	rBV	22271	32152	4.55%	0.517%
71	12.463	1864	1866	1872	rVB	6234	8706	1.23%	0.140%
72	12.530	1872	1877	1879	rBV	9793	13082	1.85%	0.210%
73	12.555	1879	1881	1888	rVV2	8295	11919	1.69%	0.192%
74	12.719	1899	1908	1913	rBV5	6556	15969	2.26%	0.257%
75	12.920	1939	1941	1945	rVV2	6736	8386	1.19%	0.135%
76	12.969	1945	1949	1955	rVB2	9490	14917	2.11%	0.240%

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77	13.030	1955	1959	1964	rBV4	3874	7811	1.11%	0.126%
78	13.268	1992	1998	2000	rBV	18305	23673	3.35%	0.381%
79	13.292	2000	2002	2007	rVB2	11195	12941	1.83%	0.208%
80	13.426	2020	2024	2032	rVB7	3932	9411	1.33%	0.151%
81	13.579	2045	2049	2054	rBV3	10178	16330	2.31%	0.263%
82	13.774	2076	2081	2088	rVB	154216	198591	28.11%	3.195%
83	13.841	2088	2092	2096	rBV2	7275	9722	1.38%	0.156%
84	14.036	2120	2124	2128	rBV2	13739	16618	2.35%	0.267%
85	14.505	2194	2201	2206	rVB7	4411	11843	1.68%	0.191%
86	14.640	2215	2223	2227	rBV	117538	160157	22.67%	2.576%
87	14.780	2239	2246	2253	rVV	95566	136250	19.28%	2.192%
88	15.206	2313	2316	2320	rVV2	11206	15289	2.16%	0.246%
89	15.377	2331	2344	2347	rBV3	15335	26931	3.81%	0.433%
90	15.408	2347	2349	2354	rVV2	6391	7990	1.13%	0.129%
91	15.481	2354	2361	2369	rVB3	25661	45926	6.50%	0.739%
92	15.615	2377	2383	2386	rBV	39636	61800	8.75%	0.994%
93	15.652	2386	2389	2397	rVB	26954	39707	5.62%	0.639%
94	15.834	2408	2419	2429	rVB2	14357	38233	5.41%	0.615%
95	15.987	2439	2444	2451	rVB3	5388	9400	1.33%	0.151%
96	16.322	2492	2499	2508	rVB2	14532	28454	4.03%	0.458%

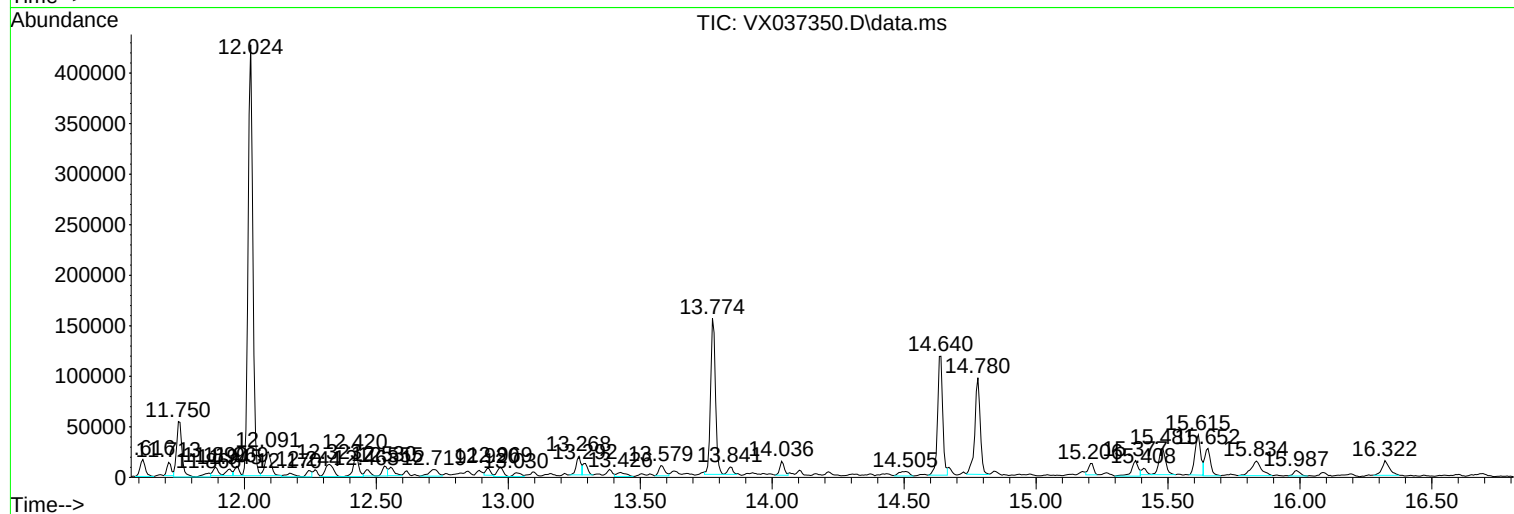
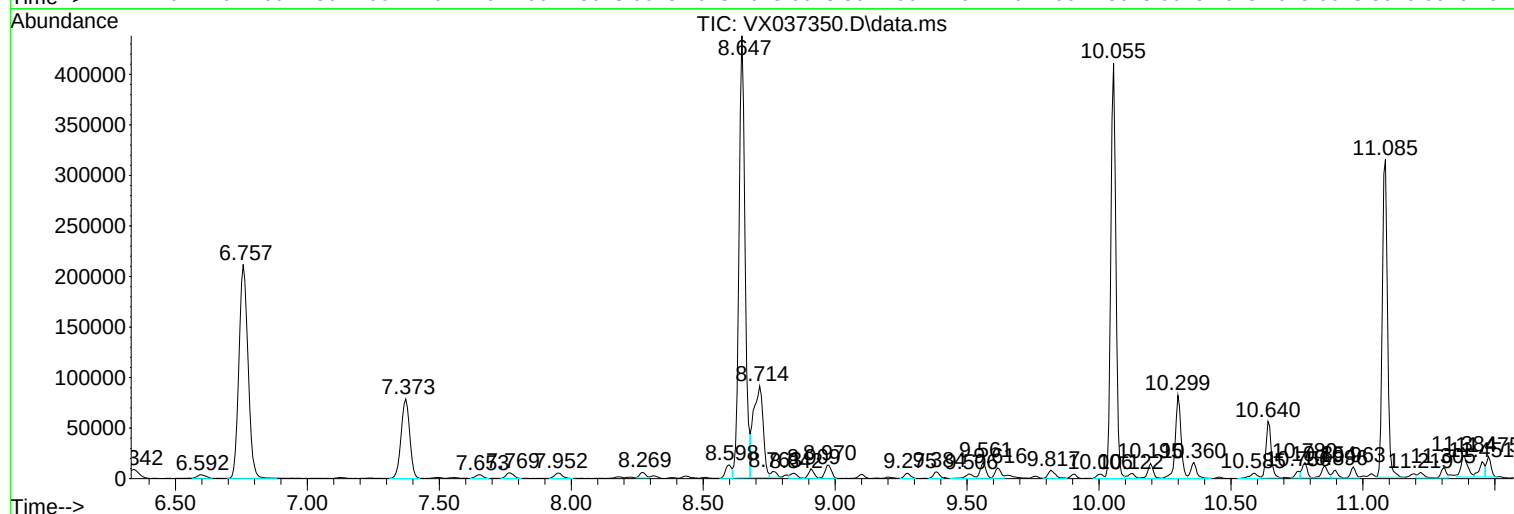
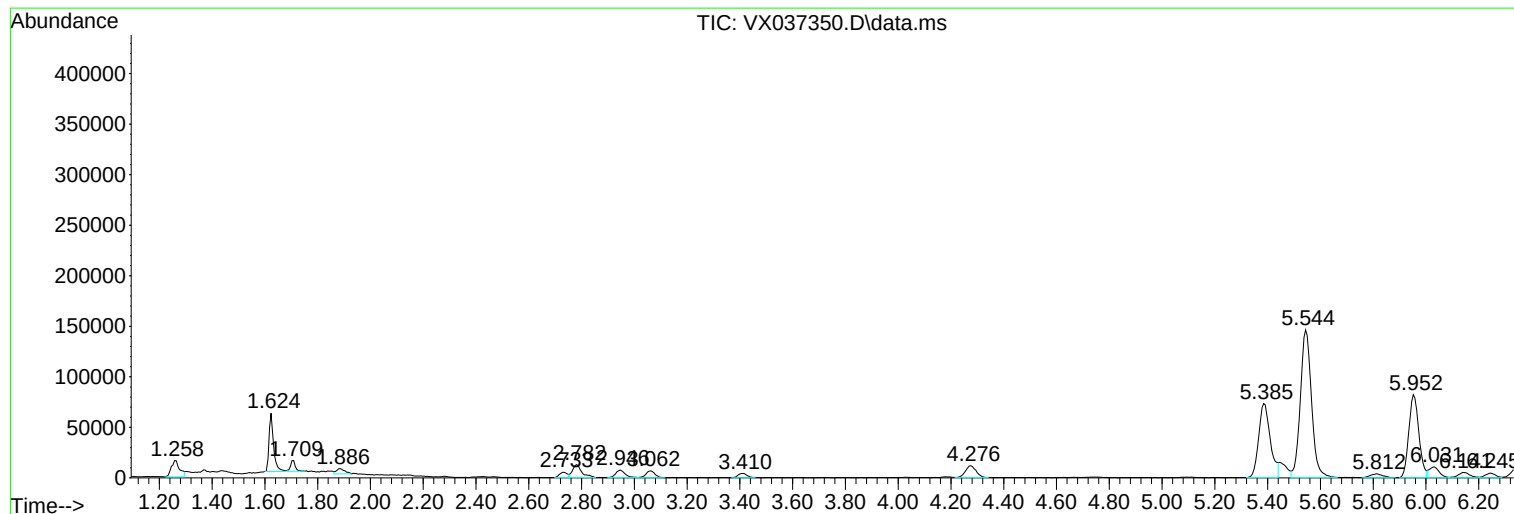
Sum of corrected areas: 6216107

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
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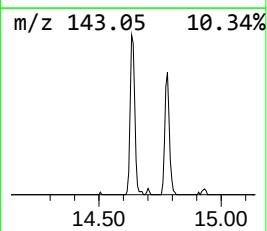
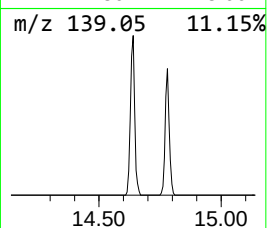
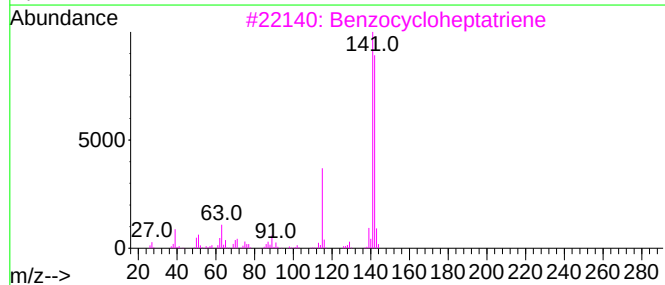
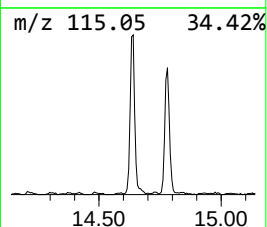
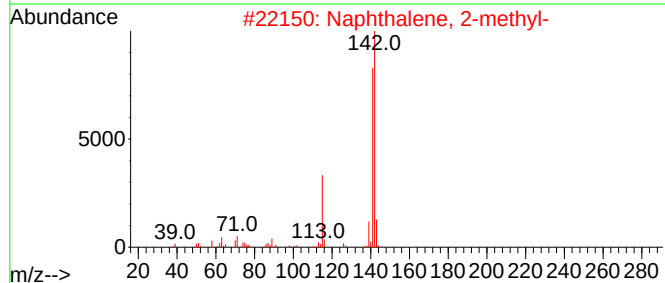
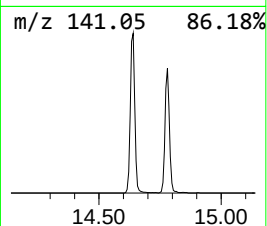
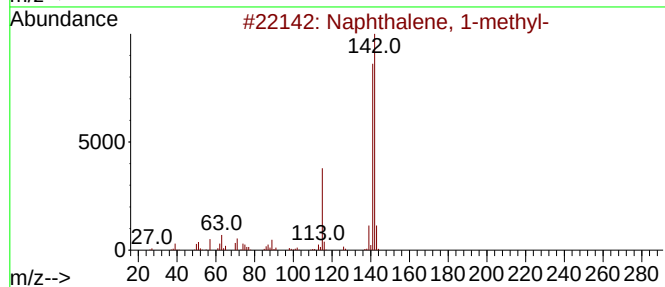
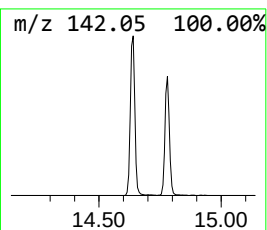
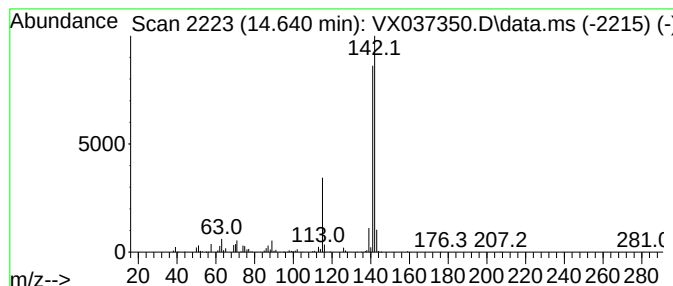
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzocycloheptatriene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	14.97 ug/l	160157	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3		Benzocycloheptatriene	142	C11H10	000264-09-5	91
4		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5		Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	78



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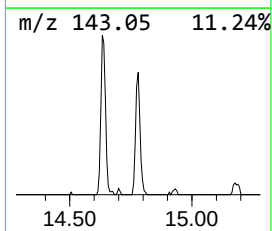
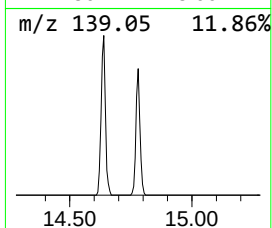
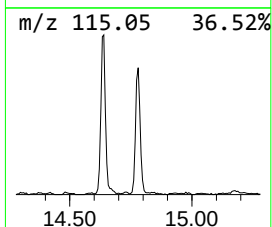
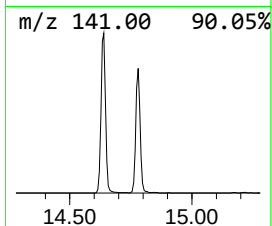
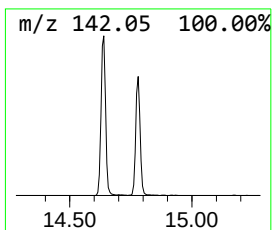
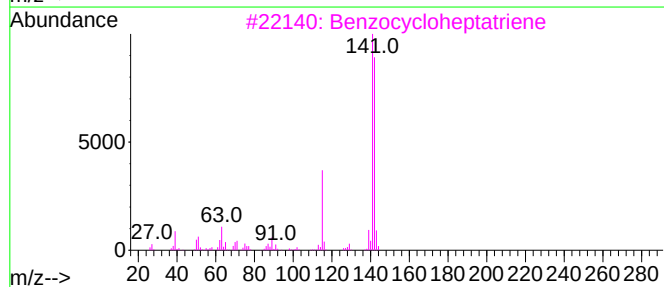
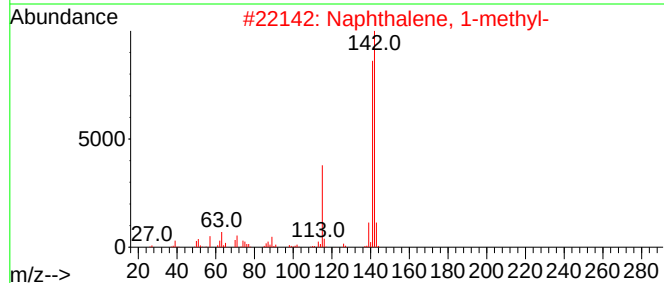
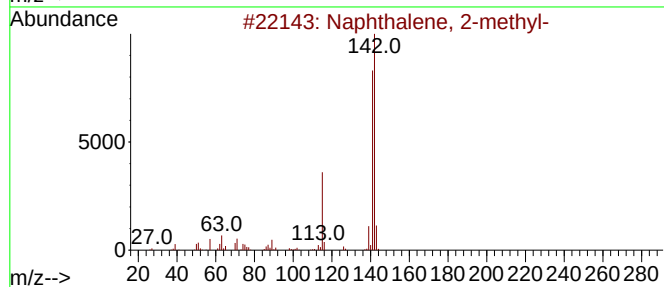
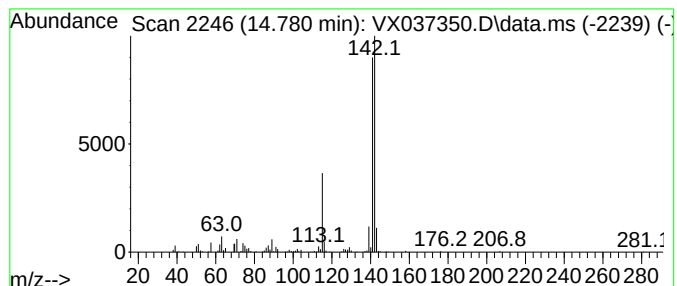
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1,4-Methanonaphthalene, 1,4... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	12.73 ug/l	136250	1,4-Dichlorobenzene-d4	12.024

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	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91



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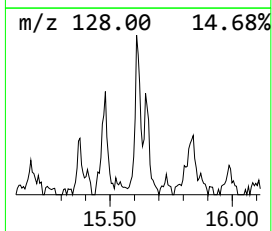
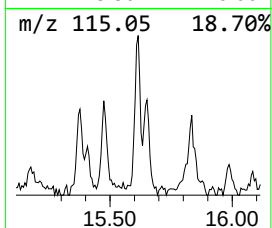
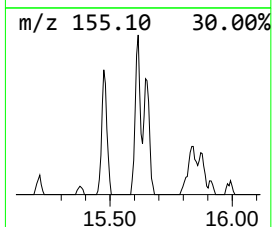
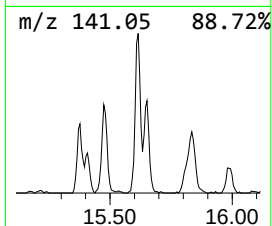
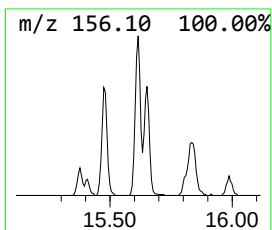
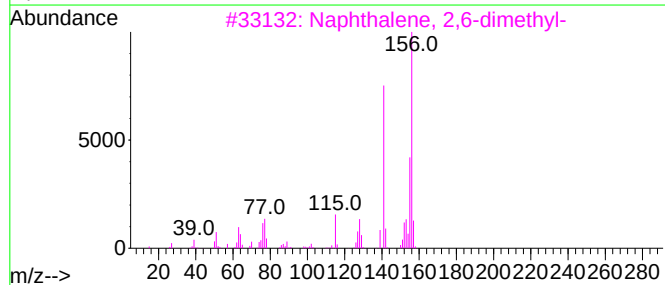
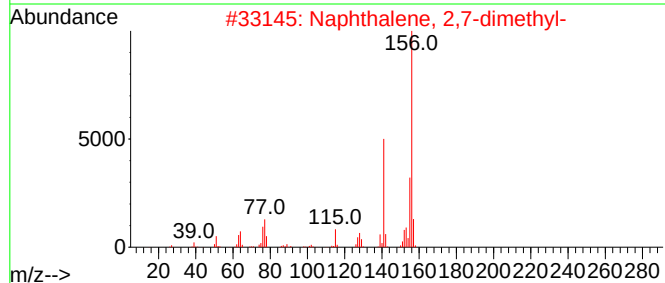
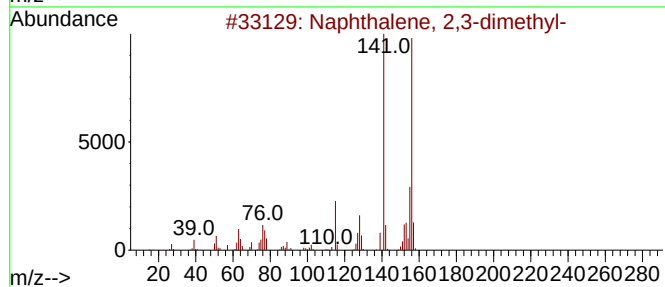
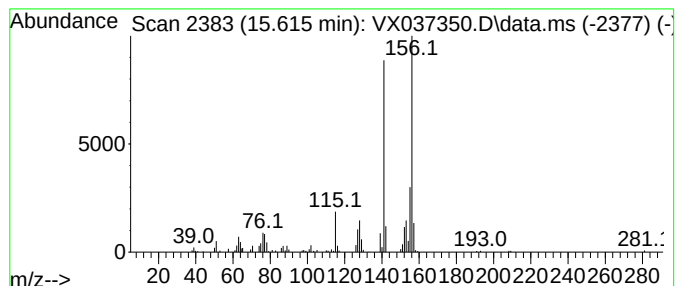
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 4 Naphthalene, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	5.78 ug/l	61800	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
4			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
5			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082923\
Data File : VX037350.D
Acq On : 29 Aug 2023 18:30
Operator : JC/MD
Sample : 04110-14
Misc : 4.78g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-21(3-4)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
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
Benzocyclohepta...	14.640	15.0	ug/l	160157	4	12.024	535049	50.0
1,4-Methanonaph...	14.780	12.7	ug/l	136250	4	12.024	535049	50.0
Naphthalene, 2,...	15.615	5.8	ug/l	61800	4	12.024	535049	50.0