

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091423\
 Data File : VX037727.D
 Acq On : 14 Sep 2023 14:07
 Operator : JC/MD
 Sample : 04374-02 20X
 Misc : 4.97g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DB-2-(26-28)

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\82X091123W.M
 Title : SW846 8260

Signal : TIC: VX037727.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.568	69	79	81	rBV6	15515	42955	3.38%	0.492%
2	4.586	564	574	584	rBV	5087	17708	1.40%	0.203%
3	5.385	693	705	720	rBV	142871	420700	33.15%	4.823%
4	5.549	720	732	752	rVB	249393	711544	56.06%	8.158%
5	5.952	788	798	820	rBV	158182	428806	33.79%	4.916%
6	6.251	837	847	857	rVB2	5296	16777	1.32%	0.192%
7	6.763	921	931	950	rBV	383037	920244	72.51%	10.551%
8	7.982	1122	1131	1140	rVB2	6821	14911	1.17%	0.171%
9	8.104	1144	1151	1160	rBV2	8329	17090	1.35%	0.196%
10	8.646	1227	1240	1255	rBV	801951	1269193	100.00%	14.551%
11	9.902	1442	1446	1451	rVB2	9836	13928	1.10%	0.160%
12	10.055	1466	1471	1488	rVB	823356	1119504	88.21%	12.835%
13	10.305	1500	1512	1517	rBV6	5552	13631	1.07%	0.156%
14	11.079	1634	1639	1650	rBV	674984	897155	70.69%	10.286%
15	11.304	1673	1676	1683	rVB	20984	28093	2.21%	0.322%
16	11.402	1686	1692	1697	rVV	14837	27485	2.17%	0.315%
17	11.457	1698	1701	1712	rVB7	6349	15399	1.21%	0.177%
18	11.750	1746	1749	1760	rVB	39564	59570	4.69%	0.683%
19	12.024	1788	1794	1800	rBV	821658	1046730	82.47%	12.001%
20	12.091	1800	1805	1812	rVB	22068	34437	2.71%	0.395%
21	12.249	1826	1831	1837	rBV	35898	53372	4.21%	0.612%
22	12.310	1837	1841	1849	rBV3	25407	47413	3.74%	0.544%
23	12.408	1851	1857	1858	rBV4	8550	12954	1.02%	0.149%
24	12.463	1862	1866	1872	rVB	26667	35163	2.77%	0.403%
25	12.530	1873	1877	1880	rBV	29357	42950	3.38%	0.492%
26	12.615	1886	1891	1894	rBV	77905	93944	7.40%	1.077%
27	12.701	1901	1905	1913	rVB3	22179	44179	3.48%	0.507%
28	12.847	1925	1929	1933	rVB	20732	27348	2.15%	0.314%
29	12.920	1935	1941	1945	rBV	46673	57258	4.51%	0.656%
30	12.963	1945	1948	1954	rVB	45542	57461	4.53%	0.659%
31	13.024	1954	1958	1964	rBV3	10719	23800	1.88%	0.273%
32	13.140	1968	1977	1978	rBV8	9641	20677	1.63%	0.237%
33	13.170	1978	1982	1986	rVB	29309	35636	2.81%	0.409%
34	13.292	1992	2002	2007	rBV2	71109	131894	10.39%	1.512%
35	13.371	2012	2015	2020	rVB2	14481	21508	1.69%	0.247%
36	13.542	2040	2043	2046	rVV2	13253	20578	1.62%	0.236%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091423\
Data File : VX037727.D
Acq On : 14 Sep 2023 14:07
Operator : JC/MD
Sample : 04374-02 20X
Misc : 4.97g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DB-2-(26-28)

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\82X091123W.M
Title : SW846 8260

37	13.578	2046	2049	2056	rVV3	25737	47962	3.78%	0.550%
38	13.670	2057	2064	2070	rVB3	15541	35740	2.82%	0.410%
39	13.774	2077	2081	2088	rVB2	10325	18441	1.45%	0.211%
40	13.847	2088	2093	2099	rVB5	10455	23313	1.84%	0.267%
41	13.926	2099	2106	2110	rBV7	15806	32771	2.58%	0.376%
42	14.036	2121	2124	2127	rVV2	11613	15845	1.25%	0.182%
43	14.072	2127	2130	2138	rVB	24151	38991	3.07%	0.447%
44	14.219	2149	2154	2160	rVB4	18158	36067	2.84%	0.414%
45	14.371	2175	2179	2183	rVB2	13283	16341	1.29%	0.187%
46	14.481	2192	2197	2203	rBV7	9850	21737	1.71%	0.249%
47	14.639	2214	2223	2227	rBV	68955	118420	9.33%	1.358%
48	14.779	2239	2246	2250	rBV2	36395	51932	4.09%	0.595%
49	14.901	2262	2266	2273	rVB5	6679	13475	1.06%	0.154%
50	15.182	2306	2312	2314	rBV2	11460	17805	1.40%	0.204%
51	15.377	2339	2344	2347	rBV	16913	28937	2.28%	0.332%
52	15.481	2355	2361	2366	rBV	40040	69202	5.45%	0.793%
53	15.615	2377	2383	2386	rBV	39240	65275	5.14%	0.748%
54	15.651	2386	2389	2397	rVB	26916	41901	3.30%	0.480%
55	15.840	2410	2420	2427	rBV3	11389	27587	2.17%	0.316%
56	15.980	2440	2443	2448	rBV3	8312	13436	1.06%	0.154%
57	16.084	2454	2460	2467	rBV	11290	20508	1.62%	0.235%
58	16.194	2475	2478	2485	rVB5	8833	14546	1.15%	0.167%
59	16.352	2499	2504	2513	rBV4	15187	33703	2.66%	0.386%
60	16.590	2539	2543	2549	rVB2	15880	28735	2.26%	0.329%
61	16.657	2549	2554	2566	rVB3	20406	47432	3.74%	0.544%

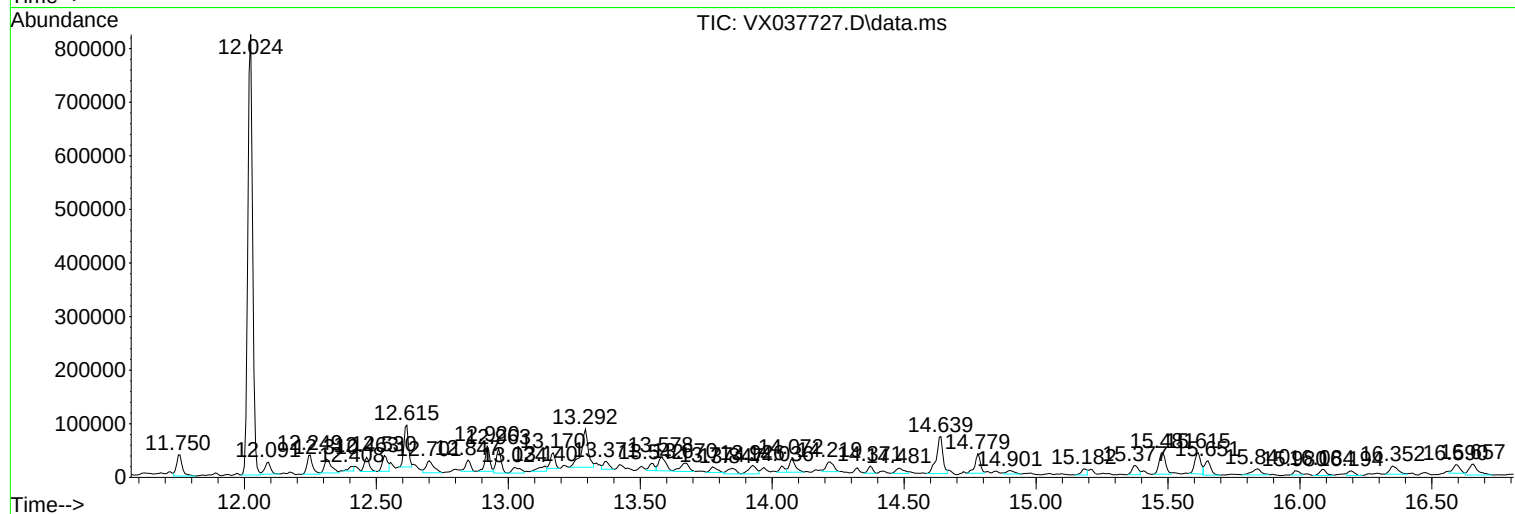
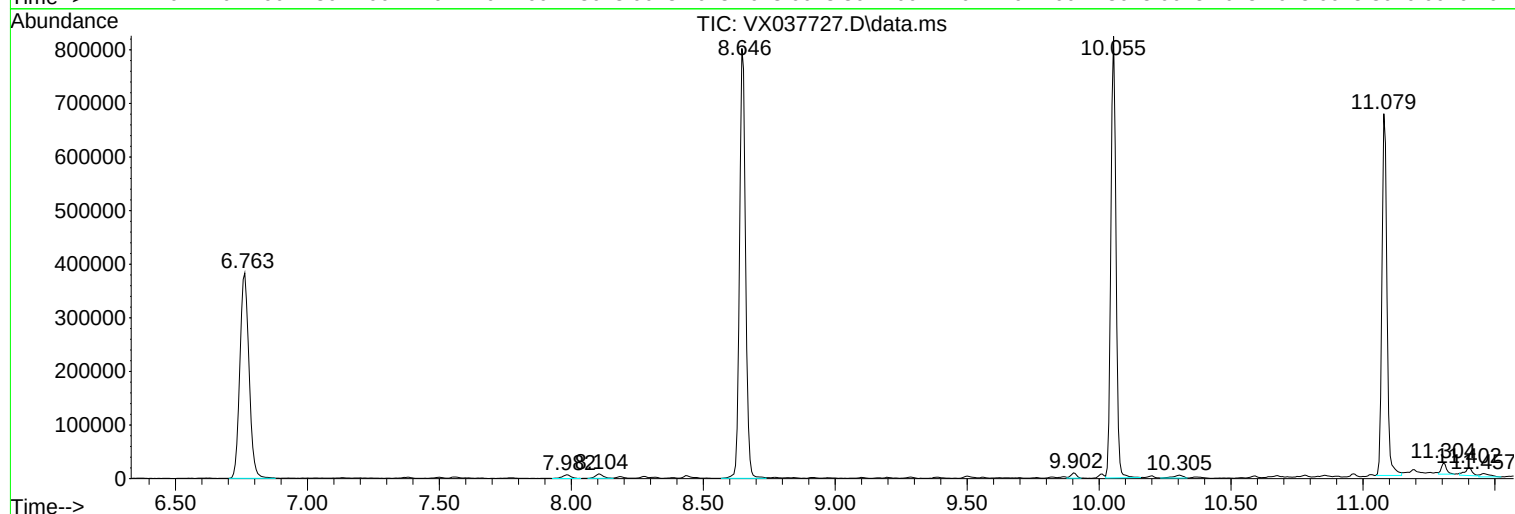
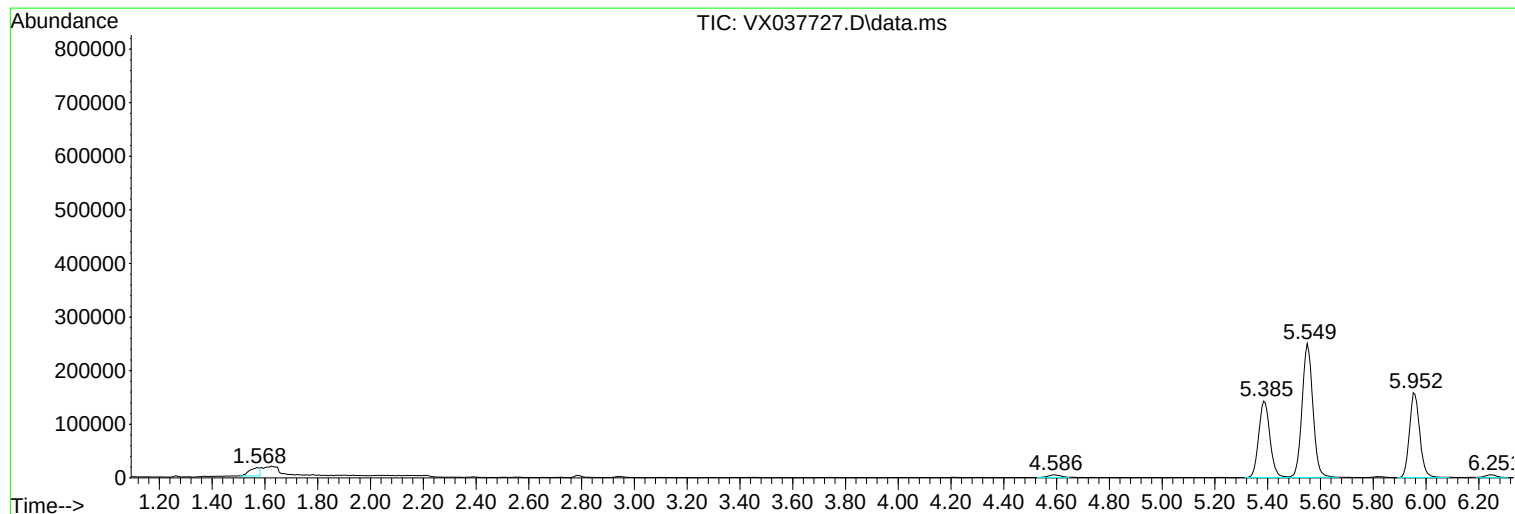
Sum of corrected areas: 8722097

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091423\
Data File : VX037727.D
Acq On : 14 Sep 2023 14:07
Operator : JC/MD
Sample : 04374-02 20X
Misc : 4.97g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DB-2-(26-28)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091123W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091423\
Data File : VX037727.D
Acq On : 14 Sep 2023 14:07
Operator : JC/MD
Sample : 04374-02 20X
Misc : 4.97g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DB-2-(26-28)

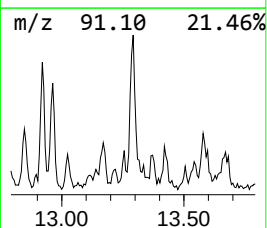
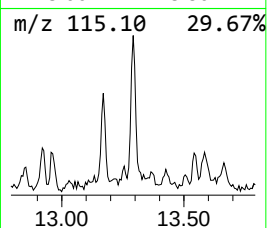
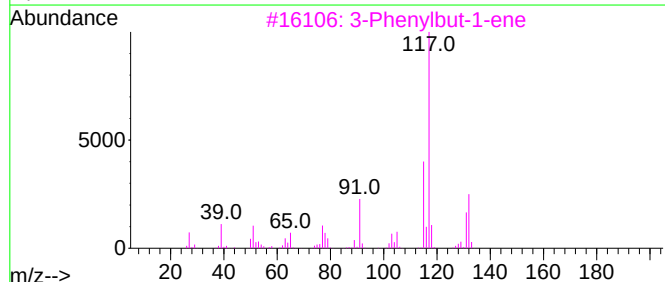
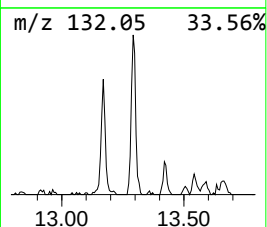
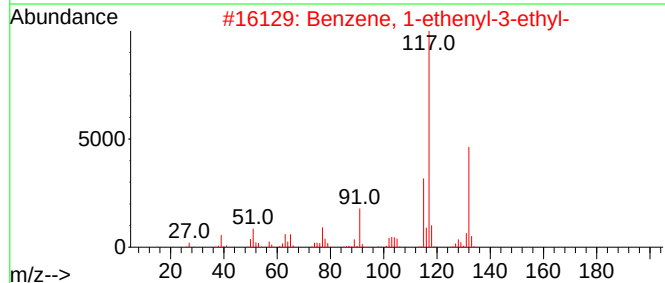
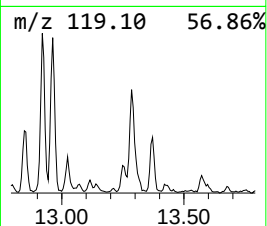
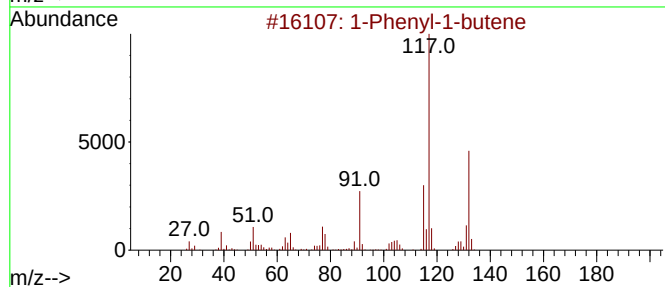
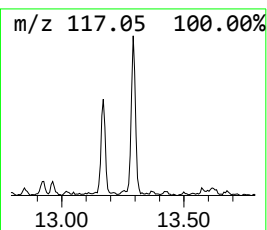
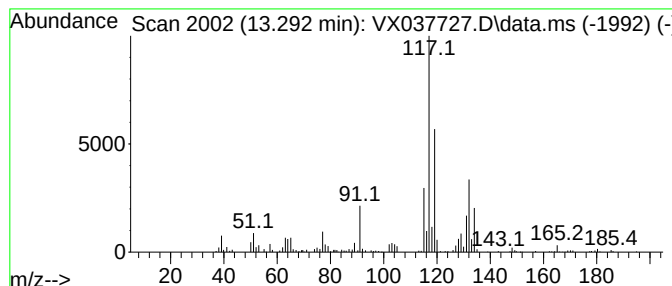
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091123W.M
Quant Title : SW846 8260

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

Peak Number 1 1-Phenyl-1-butene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	6.30 ug/l	131894	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenyl-1-butene	132	C10H12	000824-90-8	95
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	92
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
4			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	70
5			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091423\
Data File : VX037727.D
Acq On : 14 Sep 2023 14:07
Operator : JC/MD
Sample : 04374-02 20X
Misc : 4.97g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DB-2-(26-28)

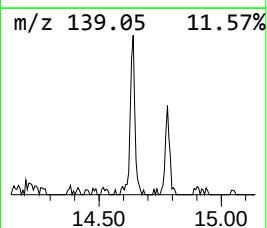
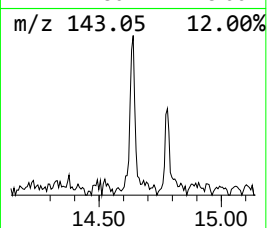
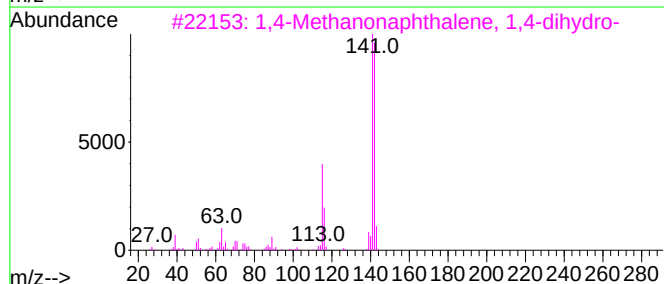
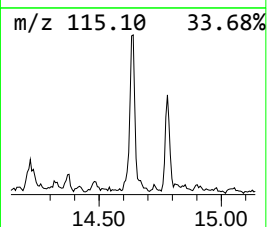
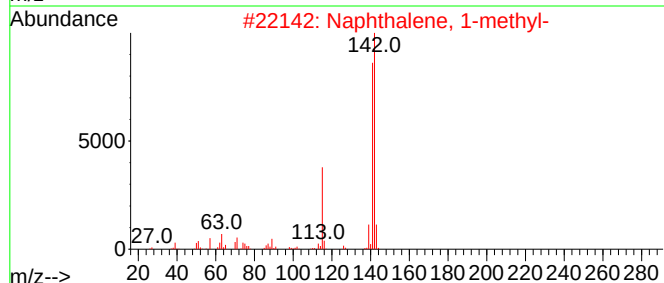
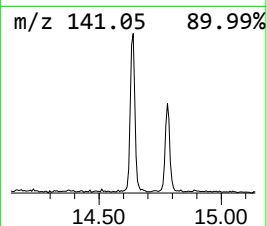
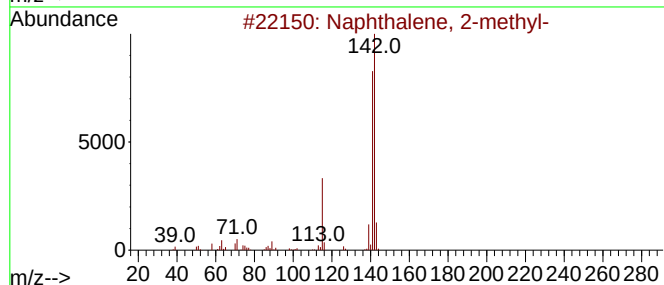
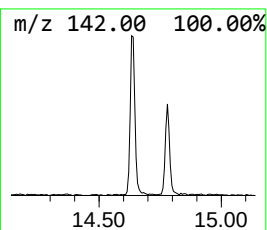
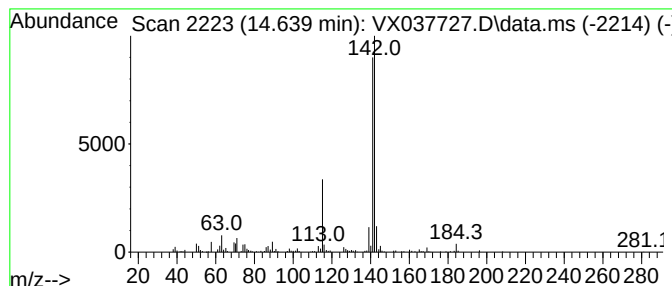
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091123W.M
Quant Title : SW846 8260

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

Peak Number 2 Naphthalene, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.639	5.66 ug/l	118420	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			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	90
5			1-Naphthaleneacetamide	185	C12H11NO	000086-86-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091423\
Data File : VX037727.D
Acq On : 14 Sep 2023 14:07
Operator : JC/MD
Sample : 04374-02 20X
Misc : 4.97g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DB-2-(26-28)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091123W.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
1-Phenyl-1-butene	13.292	6.3	ug/l	131894	4	12.024	1046730	50.0
Naphthalene, 2-...	14.639	5.7	ug/l	118420	4	12.024	1046730	50.0