

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121523\
 Data File : BM043368.D
 Acq On : 15 Dec 2023 21:24
 Operator : MA/JU
 Sample : 05794-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 BGRF7

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0.1 % 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:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BM043368.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.281	13	16	24	rVB5	22545	34651	0.71%	0.057%
2	3.387	31	34	42	rVB	43519	58712	1.21%	0.096%
3	3.828	105	109	113	rVB2	17045	21057	0.43%	0.034%
4	3.928	122	126	132	rBV	72240	94868	1.95%	0.155%
5	3.999	135	138	141	rVV2	17389	22106	0.45%	0.036%
6	4.040	141	145	152	rVB	56982	89140	1.83%	0.146%
7	4.140	157	162	173	rVB	50040	79929	1.64%	0.131%
8	4.369	196	201	210	rBV	256915	354592	7.29%	0.580%
9	4.522	223	227	231	rVB3	16823	24066	0.49%	0.039%
10	4.657	245	250	254	rBV4	17413	29538	0.61%	0.048%
11	4.710	255	259	265	rVB4	28107	40994	0.84%	0.067%
12	4.781	265	271	280	rBV	189403	287119	5.90%	0.469%
13	5.069	314	320	329	rBV	87831	138532	2.85%	0.227%
14	5.175	334	338	344	rVV3	27347	39124	0.80%	0.064%
15	5.963	467	472	481	rVB2	54076	87035	1.79%	0.142%
16	6.381	539	543	549	rBV3	13533	21427	0.44%	0.035%
17	6.440	549	553	562	rVB5	15538	31353	0.64%	0.051%
18	7.151	665	674	691	rVB3	790835	1915152	39.36%	3.132%
19	7.328	697	704	715	rBV	577717	932182	19.16%	1.524%
20	7.516	728	736	746	rBV	682355	1115048	22.92%	1.823%
21	7.604	746	751	759	rVV5	16459	40798	0.84%	0.067%
22	7.992	807	817	835	rBV	1723810	2798471	57.52%	4.576%
23	8.240	855	859	864	rVB6	17352	28594	0.59%	0.047%
24	8.698	930	937	951	rBV	732309	1237511	25.44%	2.024%
25	8.822	951	958	970	rVV	1104459	1854124	38.11%	3.032%
26	8.945	974	979	991	rVB	93745	175479	3.61%	0.287%
27	9.163	1009	1016	1027	rVV	684279	1134248	23.31%	1.855%
28	9.269	1027	1034	1039	rVV	43874	71042	1.46%	0.116%
29	9.322	1039	1043	1051	rVB6	11510	23033	0.47%	0.038%
30	9.410	1051	1058	1062	rBV5	13025	24935	0.51%	0.041%
31	9.881	1130	1138	1145	rBV	515273	879513	18.08%	1.438%
32	10.075	1156	1171	1189	rBV	508705	1455975	29.93%	2.381%
33	10.245	1193	1200	1210	rVV	257874	434227	8.92%	0.710%
34	10.363	1213	1220	1223	rBV2	18381	33305	0.68%	0.054%
35	10.416	1223	1229	1236	rVB	818280	1383662	28.44%	2.263%
36	10.663	1265	1271	1275	rVV5	22392	40815	0.84%	0.067%

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37	10.798	1286	1294	1302	rBV	2388174	4116803	84.62%	6.732%
38	10.951	1314	1320	1329	rBV2	58878	128060	2.63%	0.209%
39	11.339	1379	1386	1395	rBV	155857	286742	5.89%	0.469%
40	11.592	1423	1429	1440	rVB	126942	237624	4.88%	0.389%
41	11.839	1467	1471	1479	rVB2	18678	33217	0.68%	0.054%
42	12.169	1516	1527	1532	rBV	64102	111621	2.29%	0.183%
43	12.298	1545	1549	1552	rVV6	15164	22686	0.47%	0.037%
44	12.380	1559	1563	1568	rVB4	19950	37892	0.78%	0.062%
45	12.786	1624	1632	1638	rBV4	10355	25713	0.53%	0.042%
46	13.075	1675	1681	1688	rBV5	11753	24714	0.51%	0.040%
47	13.310	1714	1721	1725	rVB2	39055	54555	1.12%	0.089%
48	13.416	1733	1739	1741	rBV7	15258	26568	0.55%	0.043%
49	13.451	1741	1745	1751	rVV2	21805	38183	0.78%	0.062%
50	13.522	1751	1757	1762	rVV2	28207	54943	1.13%	0.090%
51	13.598	1766	1770	1776	rVV8	12689	30770	0.63%	0.050%
52	13.951	1823	1830	1834	rVV7	11953	22109	0.45%	0.036%
53	14.039	1836	1845	1854	rBV	1354502	1847528	37.97%	3.021%
54	14.316	1881	1892	1905	rBV	1548764	2328453	47.86%	3.807%
55	14.621	1936	1944	1951	rBV	3390591	4865330	100.00%	7.956%
56	14.686	1951	1955	1961	rVB	29153	45090	0.93%	0.074%
57	14.816	1971	1977	1989	rBV	386187	643411	13.22%	1.052%
58	14.980	2000	2005	2009	rBV	68372	104232	2.14%	0.170%
59	15.021	2009	2012	2022	rVB6	24554	64648	1.33%	0.106%
60	15.610	2106	2112	2119	rBV	1846148	2722460	55.96%	4.452%
61	15.668	2119	2122	2126	rVB	23539	29750	0.61%	0.049%
62	15.727	2126	2132	2140	rBV	345334	498567	10.25%	0.815%
63	16.104	2192	2196	2202	rVB7	11425	20083	0.41%	0.033%
64	16.333	2229	2235	2242	rVV8	20047	45134	0.93%	0.074%
65	16.827	2315	2319	2323	rBV	22704	30365	0.62%	0.050%
66	17.021	2346	2352	2359	rBV7	15283	32709	0.67%	0.053%
67	17.121	2363	2369	2373	rBV8	13657	27939	0.57%	0.046%
68	17.180	2376	2379	2383	rVB	17006	21808	0.45%	0.036%
69	17.362	2403	2410	2415	rBV	3466505	4782897	98.31%	7.821%
70	17.404	2415	2417	2422	rVV	364826	446406	9.18%	0.730%
71	17.462	2422	2427	2437	rVB2	1781588	2597449	53.39%	4.247%
72	17.774	2475	2480	2484	rBV2	30249	47967	0.99%	0.078%
73	17.868	2492	2496	2503	rBV2	47471	71383	1.47%	0.117%
74	18.139	2537	2542	2549	rBV2	46580	67756	1.39%	0.111%
75	18.262	2554	2563	2566	rBV2	216262	387665	7.97%	0.634%
76	18.339	2573	2576	2579	rBV2	22424	26750	0.55%	0.044%

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77	18.433	2587	2592	2596	rBV3	74527	133919	2.75%	0.219%
78	18.468	2596	2598	2602	rVB2	41962	51738	1.06%	0.085%
79	18.739	2641	2644	2648	rVB	32494	41698	0.86%	0.068%
80	18.786	2648	2652	2656	rBV5	31228	54160	1.11%	0.089%
81	18.839	2656	2661	2668	rVB	323361	433704	8.91%	0.709%
82	18.980	2682	2685	2688	rBV5	27761	36179	0.74%	0.059%
83	19.062	2695	2699	2703	rVB	170227	208149	4.28%	0.340%
84	19.104	2703	2706	2710	rBV	33991	42276	0.87%	0.069%
85	19.156	2711	2715	2718	rBV3	50157	73779	1.52%	0.121%
86	19.251	2718	2731	2732	rVV3	74282	218866	4.50%	0.358%
87	19.309	2734	2741	2755	rVV7	225991	1099808	22.61%	1.798%
88	19.415	2755	2759	2764	rVB	593931	780995	16.05%	1.277%
89	19.533	2776	2779	2783	rBV3	55293	63415	1.30%	0.104%
90	19.745	2810	2815	2819	rBV	1871290	2824694	58.06%	4.619%
91	19.845	2830	2832	2836	rBV2	24237	30904	0.64%	0.051%
92	19.921	2843	2845	2846	rBV2	26355	21126	0.43%	0.035%
93	20.062	2865	2869	2872	rBV2	41441	56453	1.16%	0.092%
94	20.268	2901	2904	2908	rBV2	60021	70813	1.46%	0.116%
95	20.368	2919	2921	2925	rVB2	44617	48300	0.99%	0.079%
96	21.256	3069	3072	3079	rBV2	242121	349862	7.19%	0.572%
97	21.539	3113	3120	3124	rBV	2888456	4184426	86.00%	6.842%
98	21.574	3124	3126	3133	rVB	276936	319919	6.58%	0.523%
99	23.797	3498	3504	3510	rBV2	1041372	2012824	41.37%	3.291%
100	23.956	3524	3531	3548	rVB	1880894	3957191	81.33%	6.471%

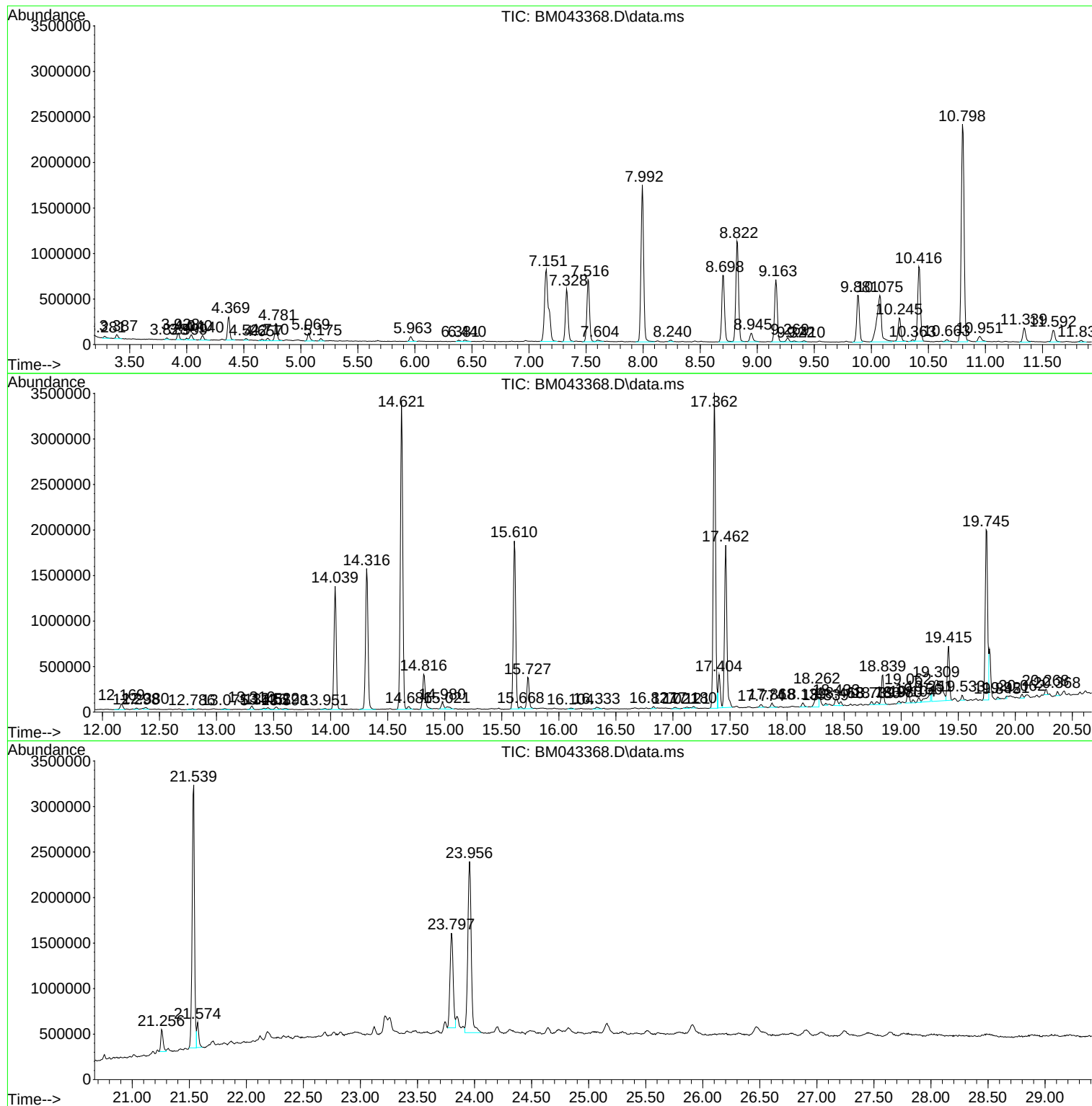
Sum of corrected areas: 61155535

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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



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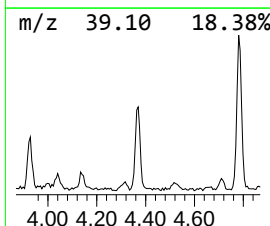
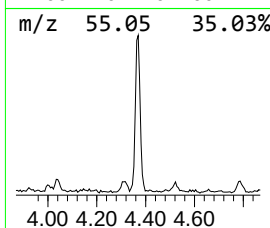
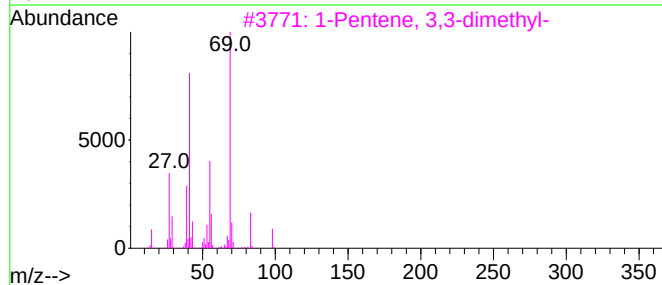
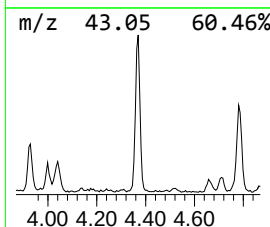
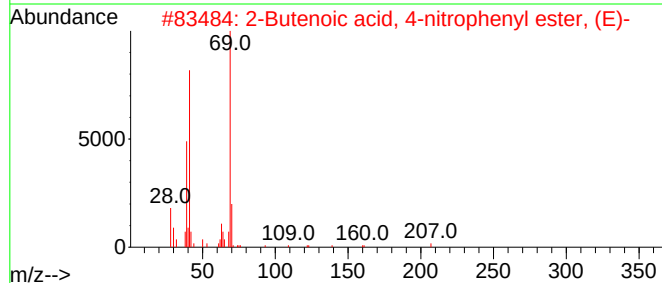
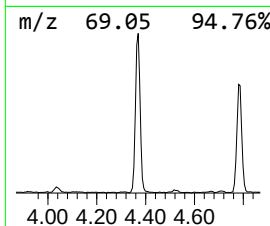
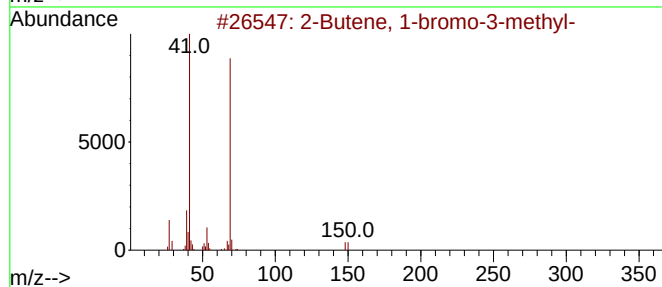
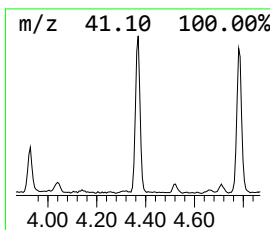
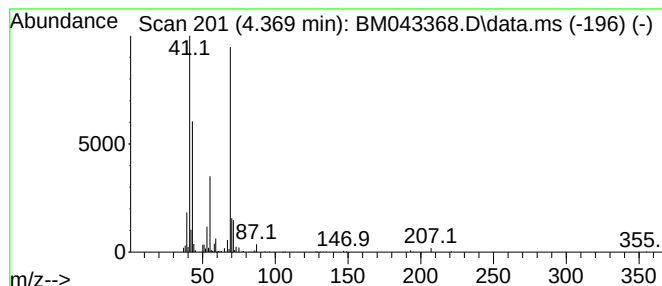
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 2-Butene, 1-bromo-3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.369	2.53 ng/ul	354592	1,4-Dichlorobenzene-d4	7.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 1-bromo-3-methyl-	148	C5H9Br	000870-63-3	59		
2	2-Butenoic acid, 4-nitrophenyl e...	207	C10H9NO4	014617-88-0	45		
3	1-Pentene, 3,3-dimethyl-	98	C7H14	003404-73-7	39		
4	1-Butene, 3,3-dimethyl-	84	C6H12	000558-37-2	39		
5	1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	38		



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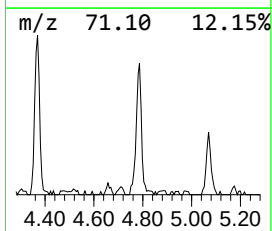
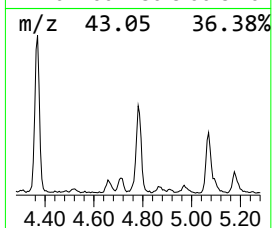
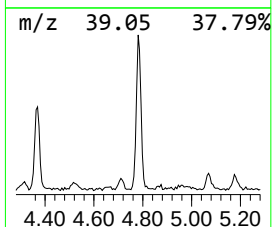
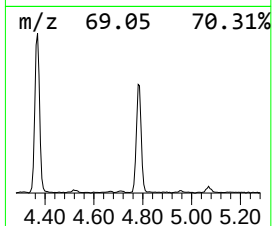
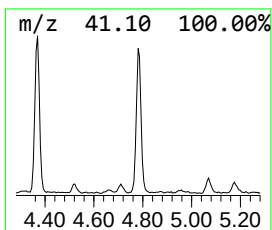
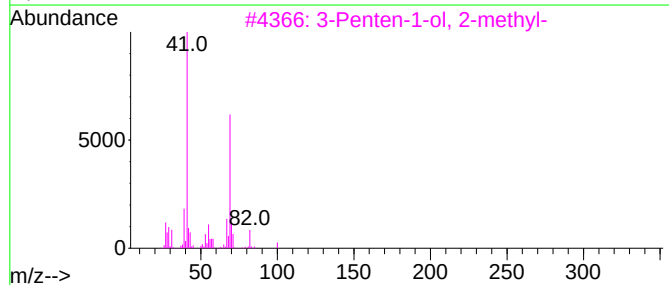
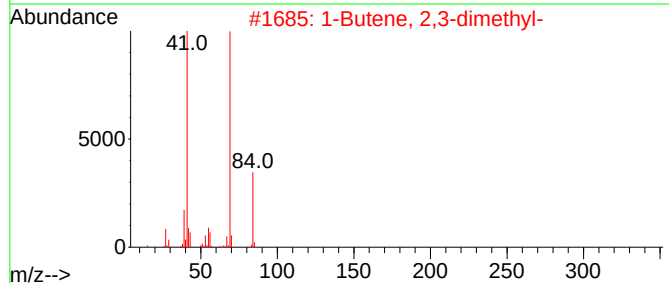
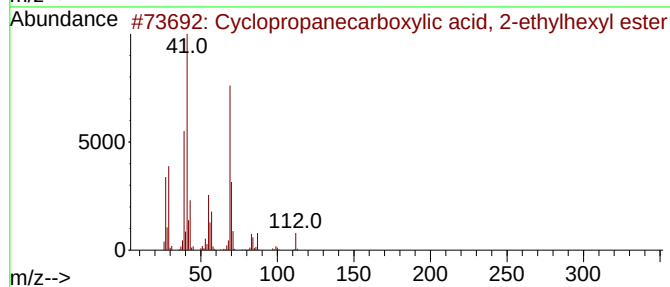
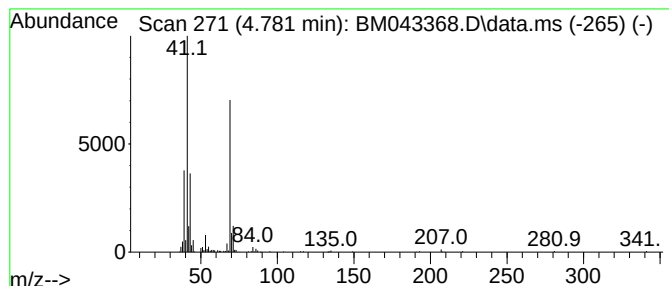
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Cyclopropanecarboxylic acid... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.781	2.05 ng/ul	287119	1,4-Dichlorobenzene-d4	7.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropanecarboxylic acid, 2-e...	198	C12H22O2	103604-31-5	50
2			1-Butene, 2,3-dimethyl-	84	C6H12	000563-78-0	50
3			3-Penten-1-ol, 2-methyl-	100	C6H12O	062238-37-3	38
4			1-Butene, 2,3-dimethyl-	84	C6H12	000563-78-0	38
5			1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	36



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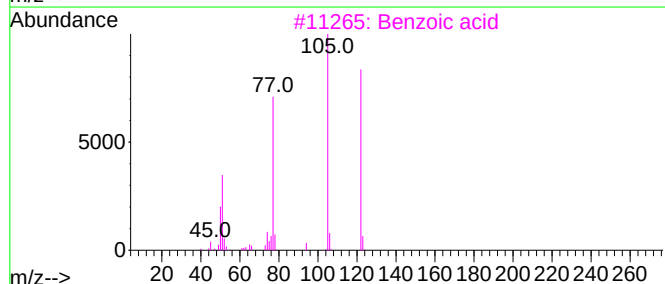
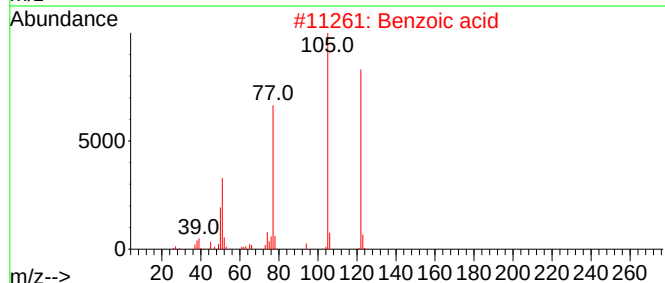
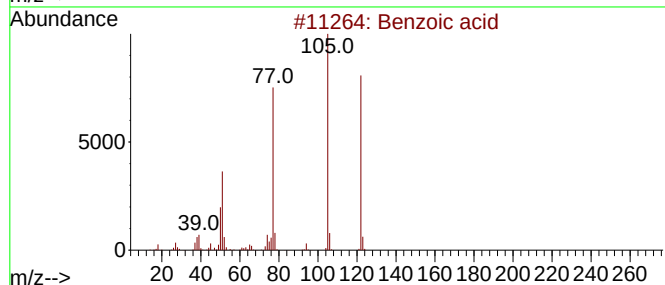
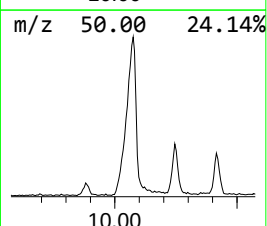
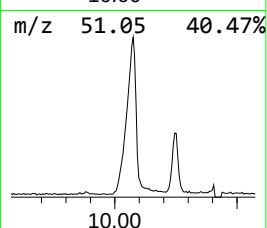
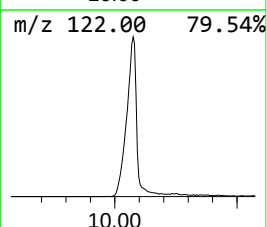
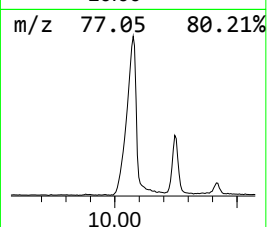
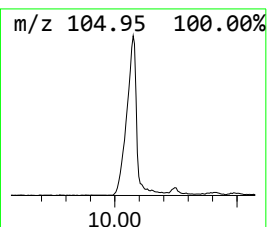
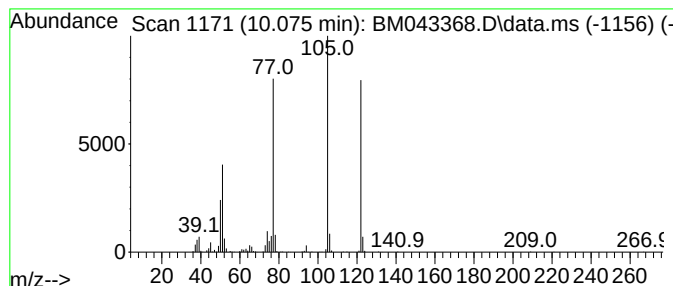
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 Benzoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.075	7.07 ng/ul	1455980	Naphthalene-d8	10.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid	122	C7H6O2	000065-85-0	96
2			Benzoic acid	122	C7H6O2	000065-85-0	96
3			Benzoic acid	122	C7H6O2	000065-85-0	96
4			Benzoic acid, silver(1+) salt	228	C7H5AgO2	000532-31-0	90
5			Heptanediamide, N,N'-di-benzoyloxy-	398	C21H22N2O6	1000253-26-4	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121523\
Data File : BM043368.D
Acq On : 15 Dec 2023 21:24
Operator : MA/JU
Sample : 05794-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BGRF7

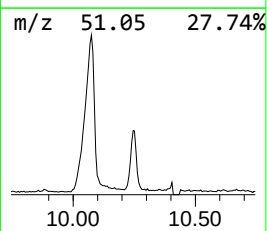
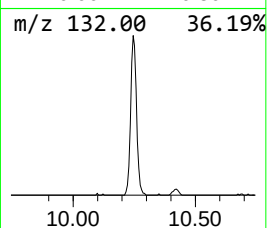
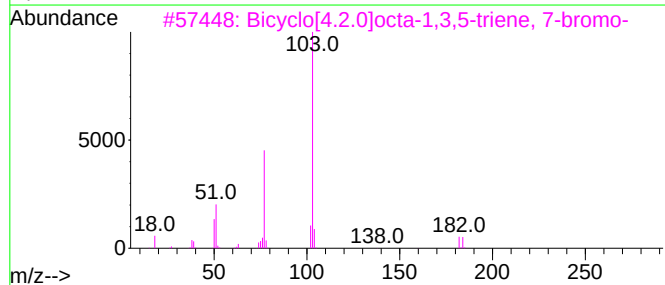
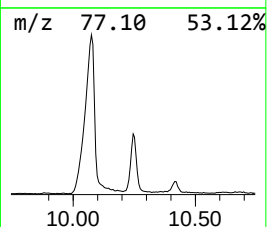
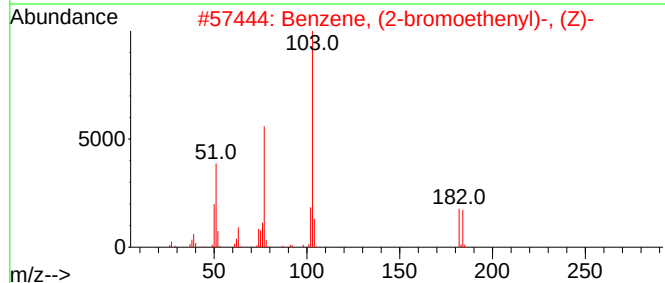
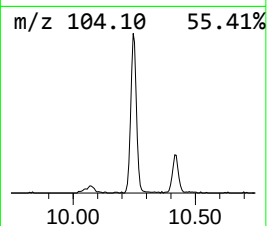
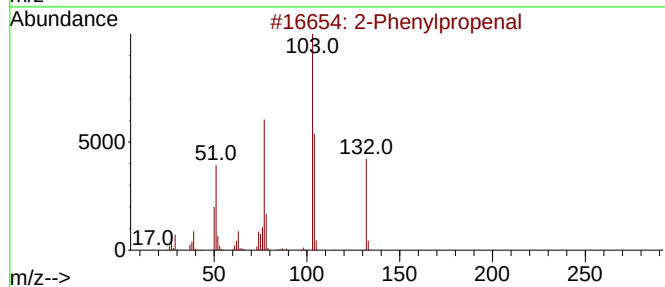
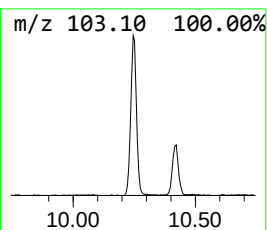
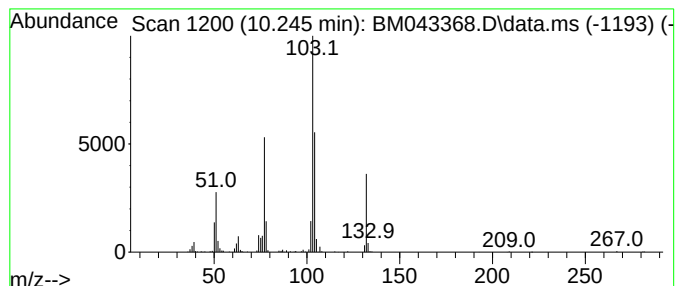
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 2-Phenylpropenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.245	2.11 ng/ul	434227	Naphthalene-d8	10.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Phenylpropenal	132	C9H8O	004432-63-7	96
2			Benzene, (2-bromoethenyl)-, (Z)-	182	C8H7Br	000588-73-8	53
3			Bicyclo[4.2.0]octa-1,3,5-triene,...	182	C8H7Br	021120-91-2	53
4			Benzene, (1-chloroethenyl)-	138	C8H7Cl	000618-34-8	47
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	182	C8H7Br	021120-91-2	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121523\
Data File : BM043368.D
Acq On : 15 Dec 2023 21:24
Operator : MA/JU
Sample : 05794-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BGRF7

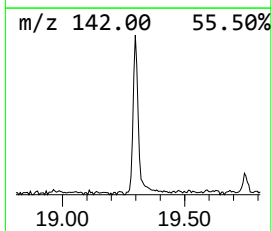
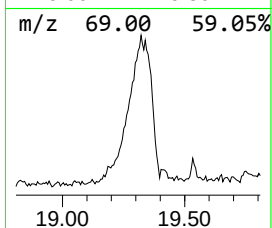
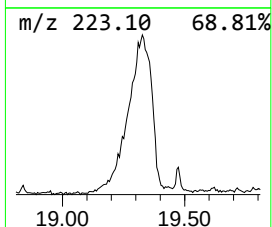
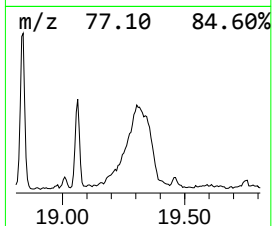
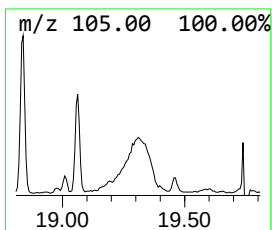
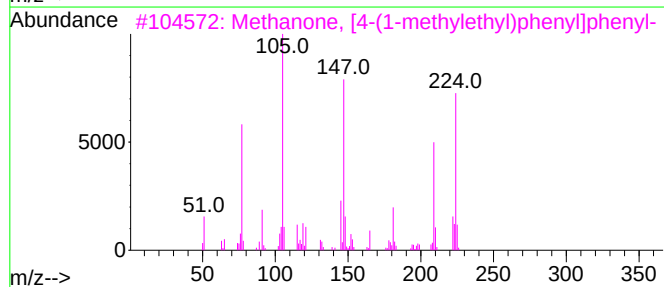
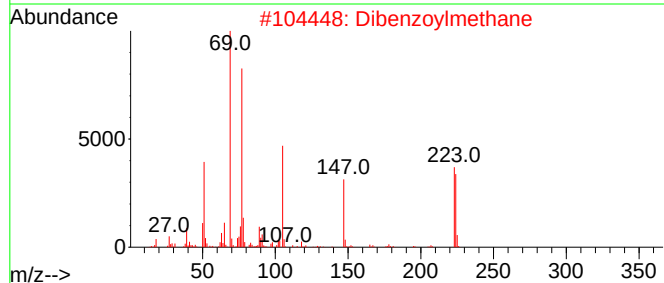
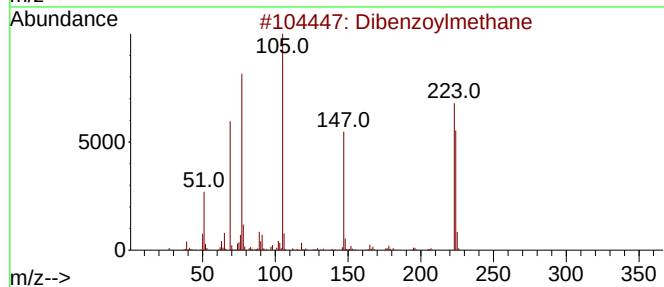
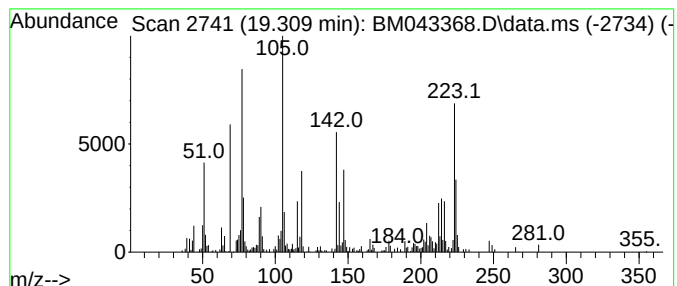
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.309	4.60 ng/ul	1099810	Phenanthrene-d10	17.362

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzoylmethane	224	C15H12O2	000120-46-7	43
2			Dibenzoylmethane	224	C15H12O2	000120-46-7	43
3			Methanone, [4-(1-methylethyl)phe...	224	C16H16O	018864-76-1	41
4			Dibenzoylmethane	224	C15H12O2	000120-46-7	38
5			Benzene, 1,4-bis(benzoylaminomet...	344	C22H20N2O2	1000295-55-1	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121523\
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Sample : 05794-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BGRF7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Butene, 1-bro...	4.369	2.5	ng/u1	354592	1	7.992	2798470	20.0
Cyclopropanecar...	4.781	2.0	ng/u1	287119	1	7.992	2798470	20.0
Benzoic acid	10.075	7.1	ng/u1	1455980	2	10.798	4116800	20.0
2-Phenylpropenal	10.245	2.1	ng/u1	434227	2	10.798	4116800	20.0
unknown-01	19.309	4.6	ng/u1	1099810	4	17.362	4782900	20.0