

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042223\
 Data File : BN025097.D
 Acq On : 23 Apr 2023 04:15
 Operator : CG/JU
 Sample : 02399-13
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 COMP1

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_N\Methods\SFAM-EPA-BN041023.M
 Title : SVOA CALIBRATION

Signal : TIC: BN025097.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.293	14	18	29	rVB	60640	84325	0.66%	0.077%
2	3.722	90	91	110	rBV	273756	524467	4.08%	0.479%
3	3.958	127	131	138	rVB5	12574	18000	0.14%	0.016%
4	4.052	143	147	154	rVB	24113	37478	0.29%	0.034%
5	4.428	208	211	220	rVB7	12586	21778	0.17%	0.020%
6	5.199	339	342	347	rBV2	15792	23912	0.19%	0.022%
7	5.434	378	382	388	rVB	18261	28807	0.22%	0.026%
8	5.952	464	470	476	rBV5	17337	30137	0.23%	0.028%
9	6.899	625	631	642	rBV8	13690	43679	0.34%	0.040%
10	7.010	646	650	652	rVV3	18677	24808	0.19%	0.023%
11	7.075	653	661	669	rVB	266786	474900	3.70%	0.434%
12	7.193	677	681	684	rBV4	7831	13327	0.10%	0.012%
13	7.246	684	690	703	rVB	1394054	2188493	17.04%	2.001%
14	7.446	717	724	734	rVV	1175424	1883654	14.66%	1.722%
15	7.534	734	739	748	rVB9	10788	21762	0.17%	0.020%
16	7.916	796	804	810	rBV	1195595	1896418	14.76%	1.734%
17	7.975	810	814	821	rVB	160403	260642	2.03%	0.238%
18	8.269	860	864	870	rVB4	13431	20815	0.16%	0.019%
19	8.475	892	899	904	rBV4	7136	17448	0.14%	0.016%
20	8.540	904	910	915	rVV2	29188	52712	0.41%	0.048%
21	8.628	918	925	936	rVV	860929	1396330	10.87%	1.276%
22	8.746	939	945	953	rVB	42272	69515	0.54%	0.064%
23	9.022	986	992	997	rBV	334468	535915	4.17%	0.490%
24	9.087	997	1003	1008	rVV	1741105	2829390	22.03%	2.586%
25	9.134	1008	1011	1023	rVV2	78083	149079	1.16%	0.136%
26	9.246	1025	1030	1038	rVB3	36804	70275	0.55%	0.064%
27	9.487	1067	1071	1081	rVB2	54447	90612	0.71%	0.083%
28	9.810	1117	1126	1140	rBV	1395241	2287083	17.81%	2.091%
29	10.040	1158	1165	1177	rVB3	21973	54418	0.42%	0.050%
30	10.246	1194	1200	1208	rBV10	9339	17861	0.14%	0.016%
31	10.346	1208	1217	1229	rBV	1828188	2990256	23.28%	2.733%
32	10.504	1239	1244	1250	rVB8	10101	18445	0.14%	0.017%
33	10.587	1252	1258	1261	rBV5	20045	33639	0.26%	0.031%
34	10.640	1261	1267	1275	rVV2	164602	316265	2.46%	0.289%
35	10.728	1275	1282	1288	rVV	1748663	2885123	22.46%	2.637%
36	10.781	1288	1291	1297	rVV	78179	123435	0.96%	0.113%

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Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.M
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37	10.869	1297	1306	1320	rVV	1792003	3058789	23.81%	2.796%
38	10.957	1320	1321	1332	rVB7	11675	20260	0.16%	0.019%
39	11.263	1368	1373	1380	rBV6	7360	14530	0.11%	0.013%
40	11.393	1390	1395	1403	rVB	24467	50847	0.40%	0.046%
41	11.522	1411	1417	1428	rVB2	71699	140945	1.10%	0.129%
42	11.722	1445	1451	1454	rBV6	8840	16138	0.13%	0.015%
43	11.898	1476	1481	1486	rBV	46430	76844	0.60%	0.070%
44	12.010	1491	1500	1515	rVV2	319251	608987	4.74%	0.557%
45	12.316	1543	1552	1561	rBV2	45805	81559	0.63%	0.075%
46	12.763	1624	1628	1637	rBV2	11027	18742	0.15%	0.017%
47	12.857	1637	1644	1648	rVV9	13186	30508	0.24%	0.028%
48	12.916	1648	1654	1664	rVV5	15612	34430	0.27%	0.031%
49	13.022	1668	1672	1676	rVV4	9403	15629	0.12%	0.014%
50	13.169	1692	1697	1701	rBV2	12236	17457	0.14%	0.016%
51	13.487	1741	1751	1766	rBV	1387503	2069063	16.11%	1.891%
52	13.604	1766	1771	1779	rVB	49031	83363	0.65%	0.076%
53	13.975	1827	1834	1848	rVB	4109646	5655525	44.03%	5.170%
54	14.087	1848	1853	1859	rVV9	8187	15583	0.12%	0.014%
55	14.257	1875	1882	1893	rBV	4385259	6347607	49.42%	5.803%
56	14.345	1893	1897	1903	rVV2	23384	44037	0.34%	0.040%
57	14.422	1906	1910	1920	rVB	41922	77969	0.61%	0.071%
58	14.563	1926	1934	1942	rVV	2822620	4042754	31.47%	3.696%
59	14.640	1942	1947	1957	rVB	53729	85078	0.66%	0.078%
60	14.757	1962	1967	1975	rBV	231402	408509	3.18%	0.373%
61	14.969	2000	2003	2010	rVB9	13258	21698	0.17%	0.020%
62	15.234	2041	2048	2055	rBV	110278	164471	1.28%	0.150%
63	15.363	2063	2070	2078	rVB5	21795	53406	0.42%	0.049%
64	15.557	2095	2103	2111	rBV	5679938	8124822	63.25%	7.427%
65	15.675	2117	2123	2136	rBV	2236447	2838594	22.10%	2.595%
66	15.792	2139	2143	2147	rVV2	31744	53584	0.42%	0.049%
67	15.839	2149	2151	2156	rVV6	10897	13367	0.10%	0.012%
68	15.922	2159	2165	2174	rVB	65100	103364	0.80%	0.094%
69	16.128	2196	2200	2205	rBV7	23408	37203	0.29%	0.034%
70	16.904	2328	2332	2337	rBV3	12186	16615	0.13%	0.015%
71	16.986	2342	2346	2351	rVB7	9674	14838	0.12%	0.014%
72	17.310	2395	2401	2408	rVB	3567593	4965104	38.65%	4.539%
73	17.410	2411	2418	2432	rBV	6636644	9283414	72.27%	8.486%
74	17.592	2444	2449	2454	rVB2	18615	27614	0.21%	0.025%
75	17.698	2461	2467	2472	rVB6	12875	23511	0.18%	0.021%
76	17.892	2496	2500	2505	rBV7	15626	26133	0.20%	0.024%

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 Title : SVOA CALIBRATION

77	17.980	2509	2515	2520	rBV	1264123	1567332	12.20%	1.433%
78	18.145	2540	2543	2547	rVB3	22385	26127	0.20%	0.024%
79	18.198	2547	2552	2561	rBV	74763	120405	0.94%	0.110%
80	18.280	2562	2566	2568	rBV2	23263	34377	0.27%	0.031%
81	18.410	2584	2588	2592	rBV2	20926	25346	0.20%	0.023%
82	18.457	2592	2596	2600	rVB2	33782	38543	0.30%	0.035%
83	18.698	2634	2637	2646	rVB2	15687	27443	0.21%	0.025%
84	18.786	2648	2652	2657	rBV8	13641	21196	0.17%	0.019%
85	19.269	2729	2734	2739	rBV2	88567	122837	0.96%	0.112%
86	19.339	2741	2746	2751	rVV	88000	126769	0.99%	0.116%
87	19.475	2765	2769	2773	rBV	69152	88289	0.69%	0.081%
88	19.627	2791	2795	2798	rVB2	29557	32914	0.26%	0.030%
89	19.704	2802	2808	2814	rBV	8330649	11172201	86.98%	10.213%
90	19.933	2844	2847	2851	rVB5	28133	32320	0.25%	0.030%
91	20.669	2969	2972	2975	rBV4	38517	40333	0.31%	0.037%
92	20.704	2975	2978	2986	rVV3	87857	135930	1.06%	0.124%
93	21.498	3108	3113	3123	rBV	4754954	5808017	45.22%	5.309%
94	22.610	3299	3302	3307	rVB	127478	171669	1.34%	0.157%
95	23.786	3493	3502	3516	rBV2	5793406	12845111	100.00%	11.742%
96	23.939	3521	3528	3543	rVV2	3453215	6638975	51.68%	6.069%

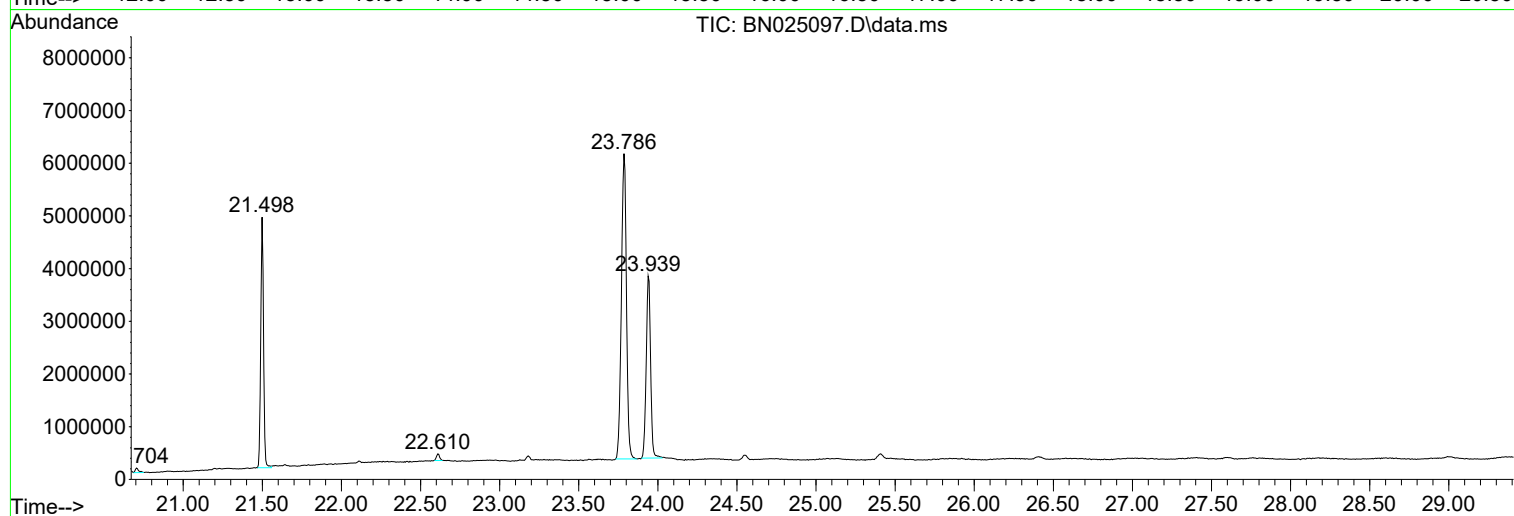
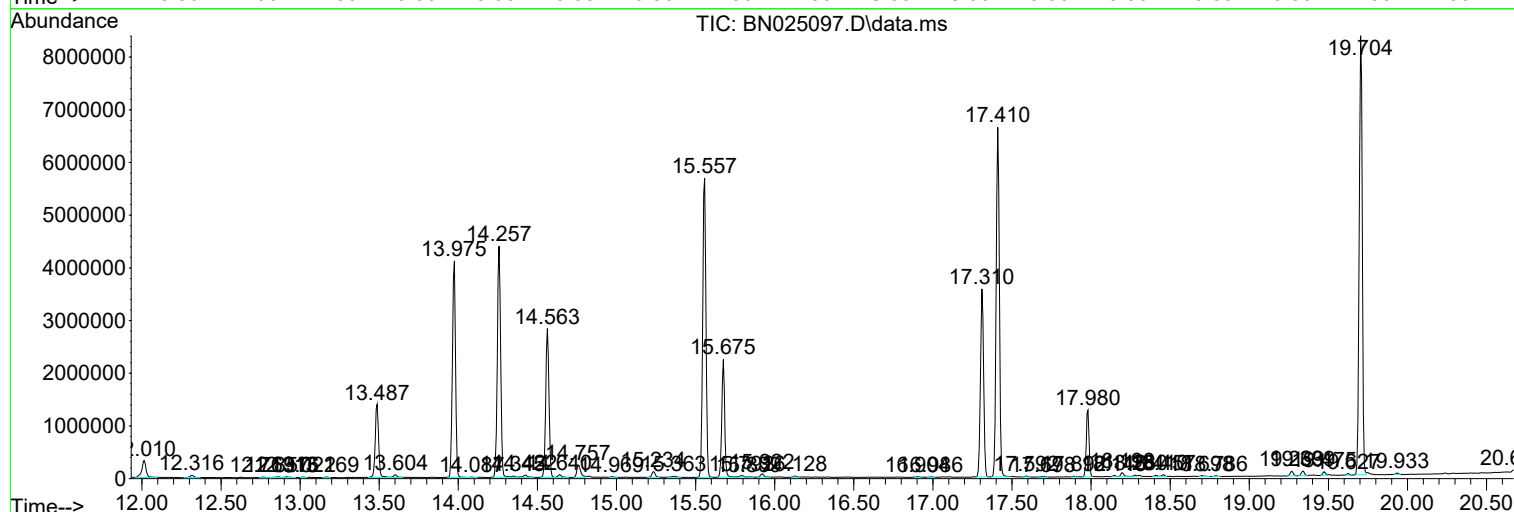
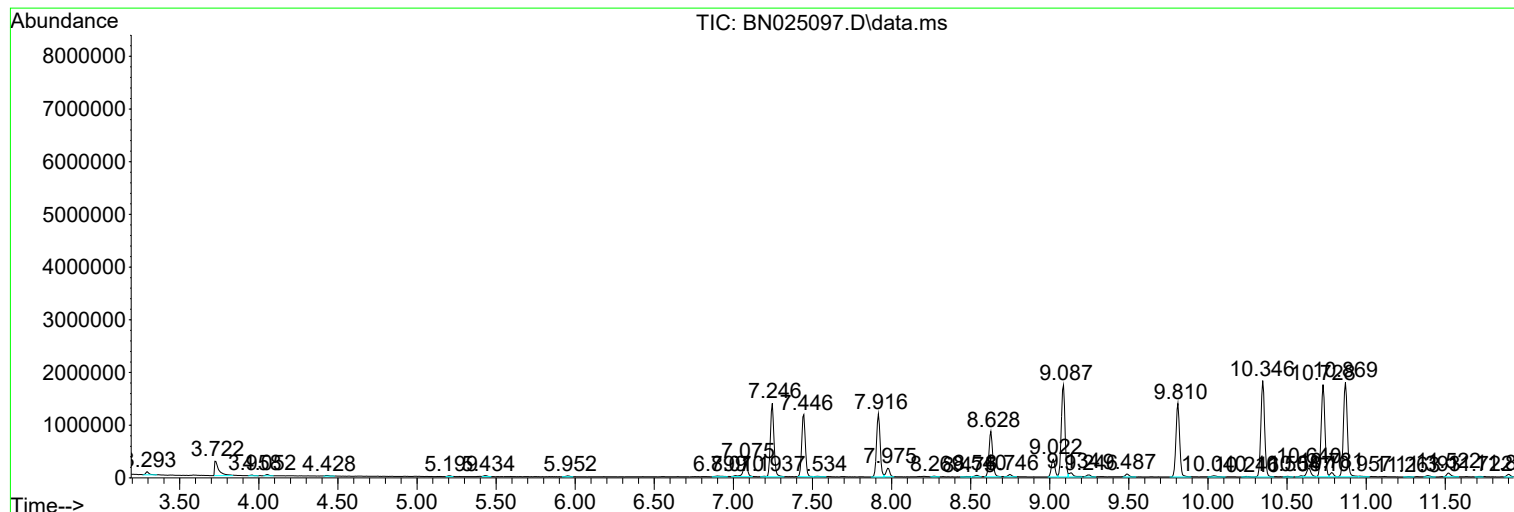
Sum of corrected areas: 109394228

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.M
Quant Title : SVOA CALIBRATION

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



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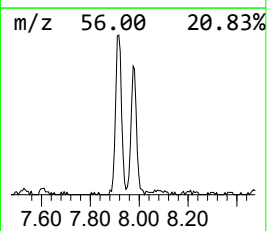
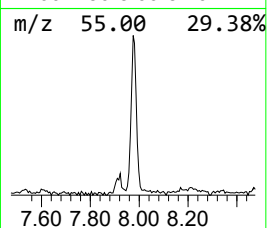
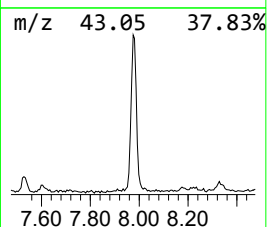
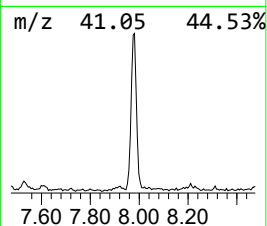
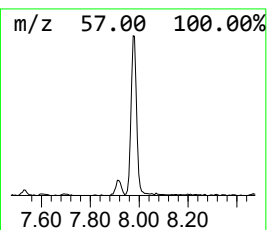
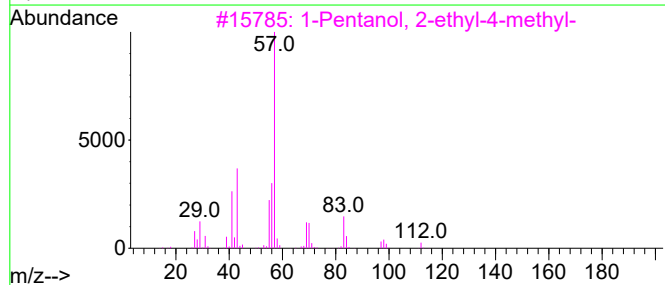
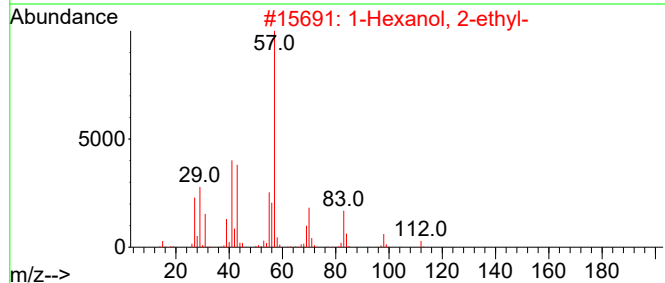
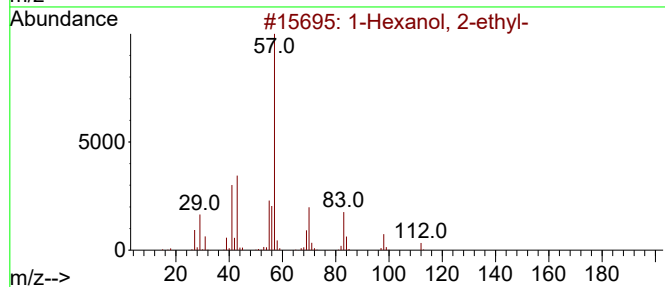
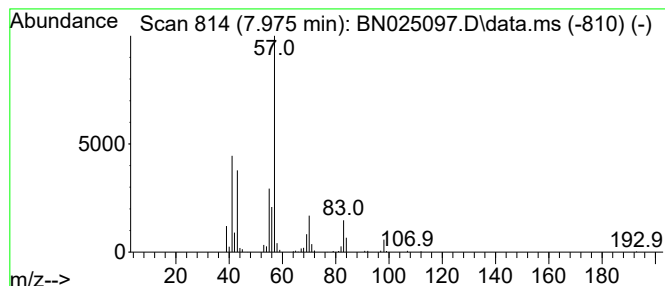
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.975	2.75 ng/ul	260642	1,4-Dichlorobenzene-d4	7.916

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
4		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	53



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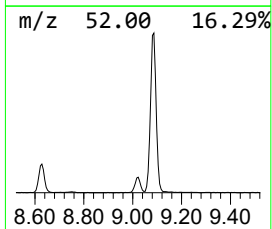
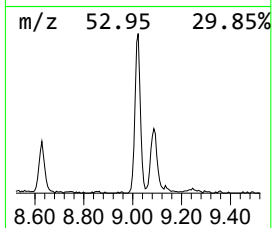
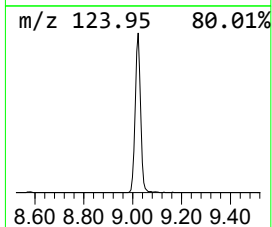
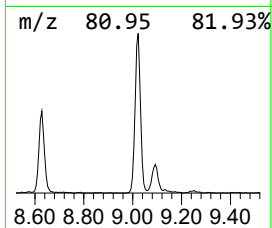
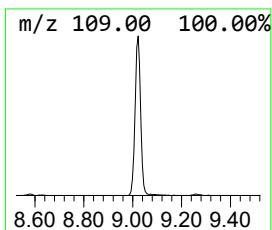
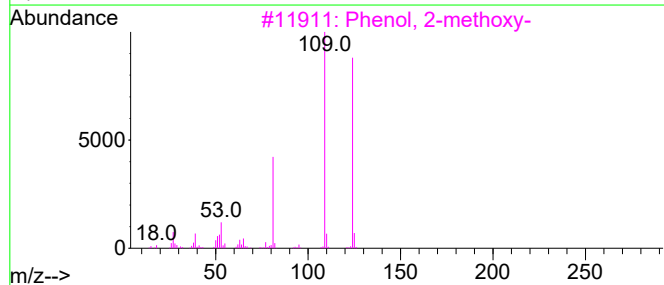
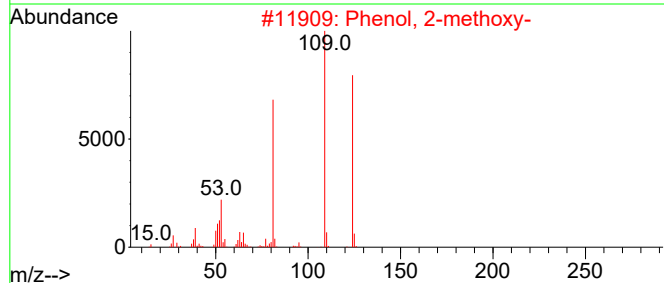
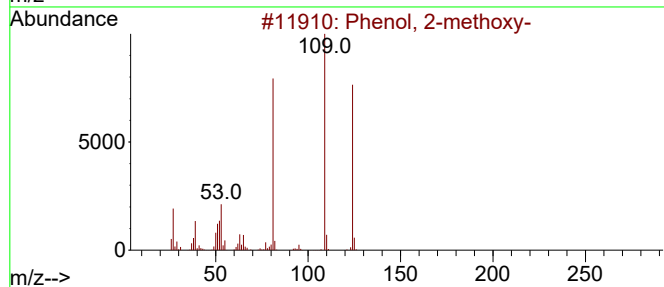
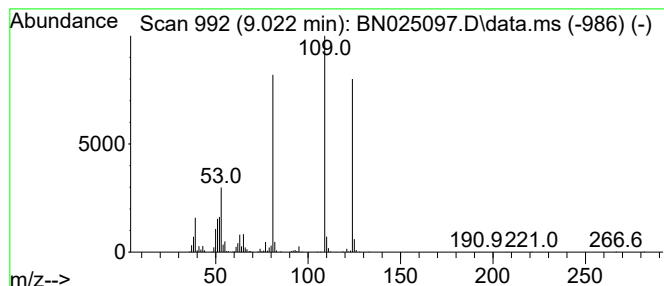
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Phenol, 2-methoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.022	5.65 ng/ul	535915	1,4-Dichlorobenzene-d4	7.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	97
2			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	96
3			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	94
4			Mequinol	124	C7H8O2	000150-76-5	91
5			Mequinol	124	C7H8O2	000150-76-5	90



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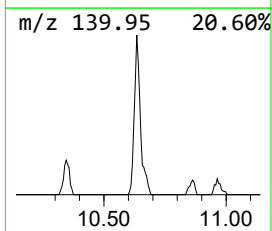
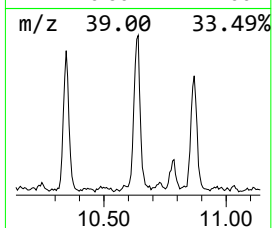
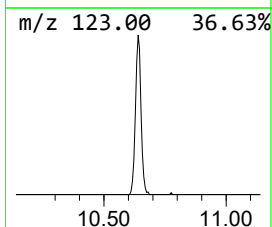
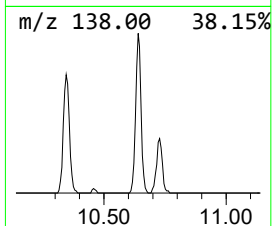
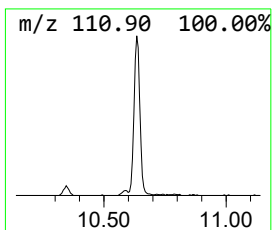
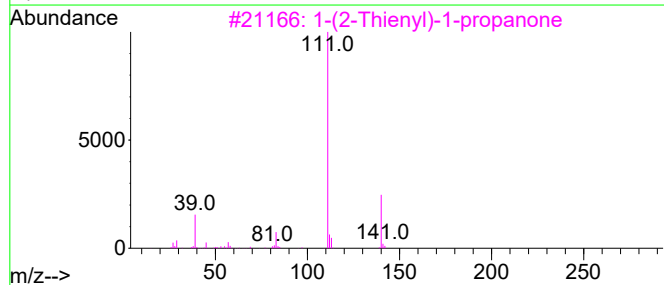
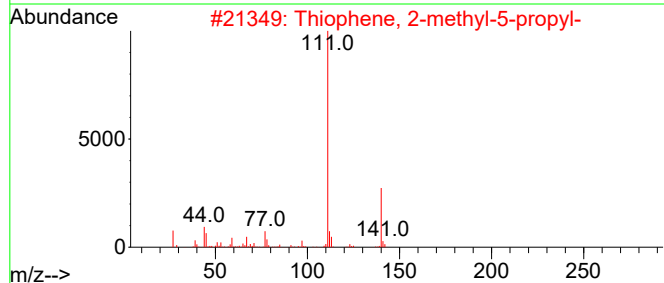
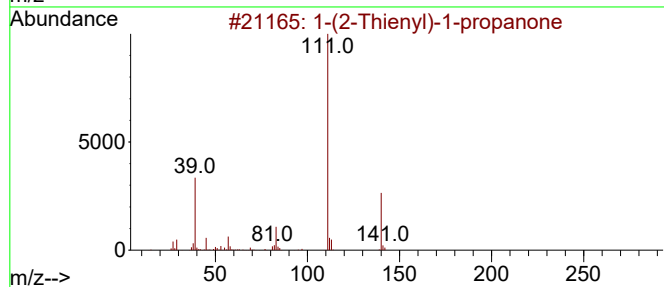
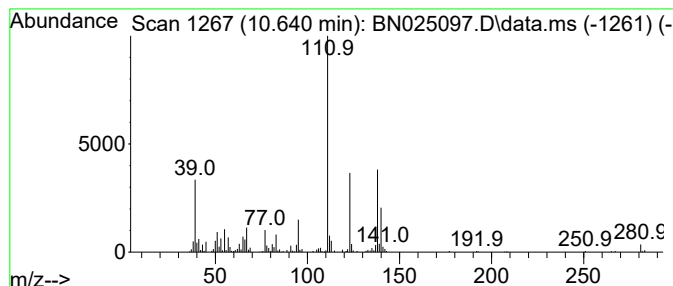
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 1-(2-Thienyl)-1-propanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.640	2.19 ng/ul	316265	Naphthalene-d8	10.728

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-(2-Thienyl)-1-propanone	140	C7H8OS	013679-75-9	55
2			Thiophene, 2-methyl-5-propyl-	140	C8H12S	033933-73-2	49
3			1-(2-Thienyl)-1-propanone	140	C7H8OS	013679-75-9	46
4			Glycine, N-(2-thienylcarbonyl)-,...	199	C8H9NO3S	1000299-60-2	43
5			N-(4-Chlorophenyl)thiophene-2-ca...	237	C11H8ClNOS	015950-35-3	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042223\
Data File : BN025097.D
Acq On : 23 Apr 2023 04:15
Operator : CG/JU
Sample : 02399-13
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
COMP1

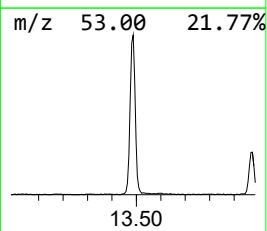
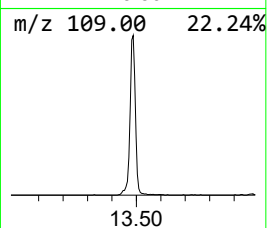
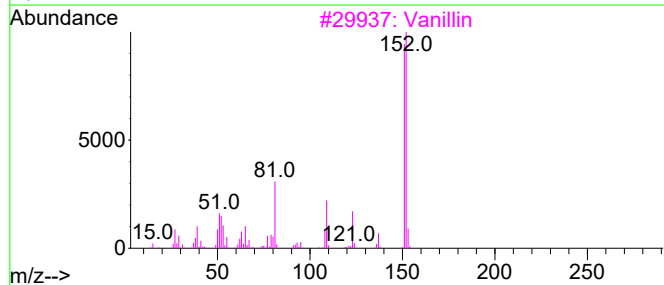
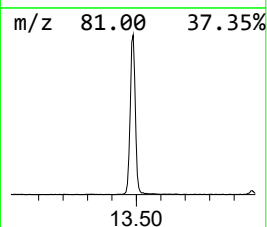
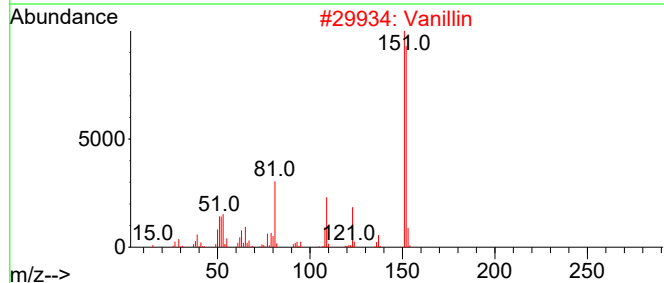
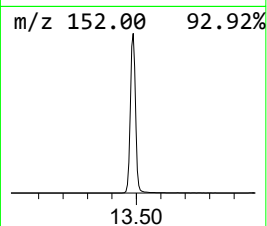
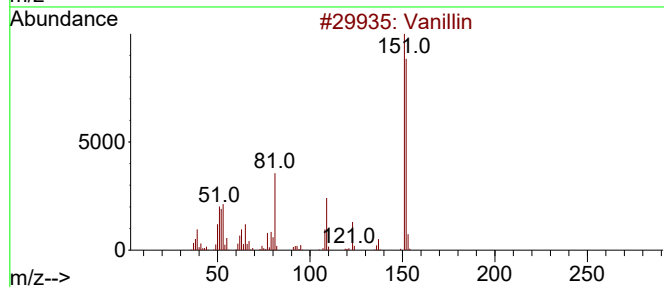
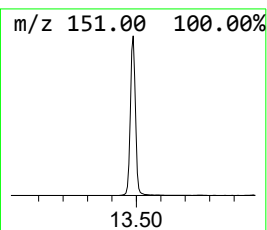
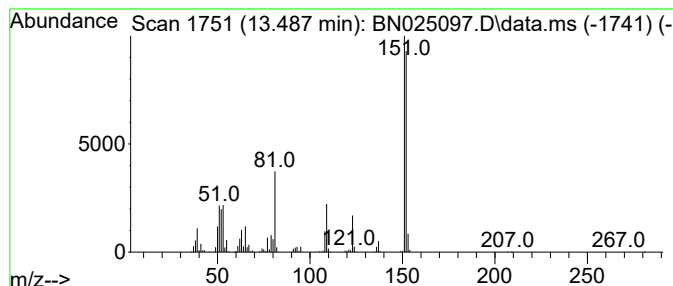
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Vanillin Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.487	10.24 ng/ul	2069060	Acenaphthene-d10	14.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin			152	C8H8O3	000121-33-5	98
2	Vanillin			152	C8H8O3	000121-33-5	97
3	Vanillin			152	C8H8O3	000121-33-5	97
4	Benzaldehyde, 3-hydroxy-4-methoxy-			152	C8H8O3	000621-59-0	97
5	Benzaldehyde, 3-hydroxy-4-methoxy-			152	C8H8O3	000621-59-0	97



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042223\
Data File : BN025097.D
Acq On : 23 Apr 2023 04:15
Operator : CG/JU
Sample : 02399-13
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
COMP1

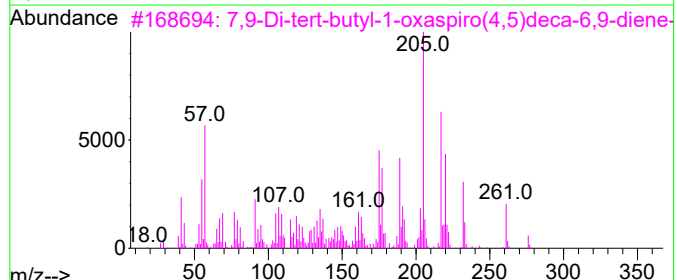
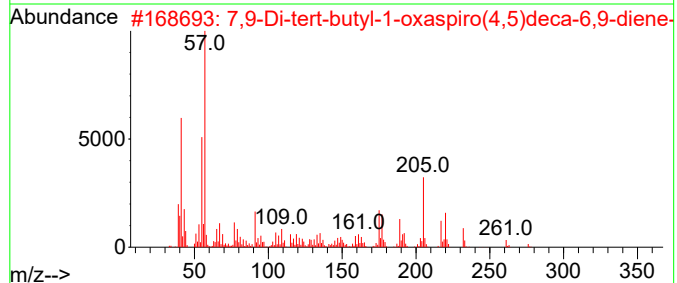
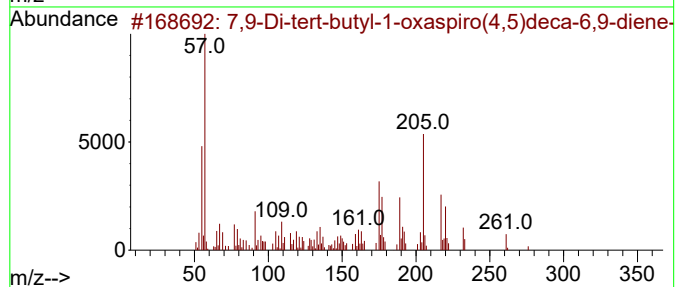
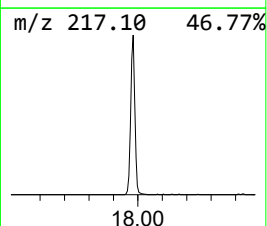
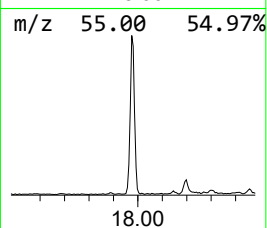
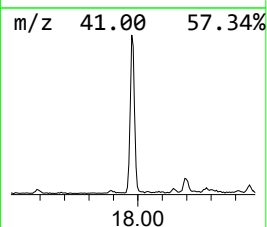
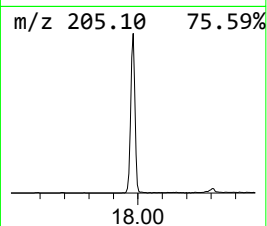
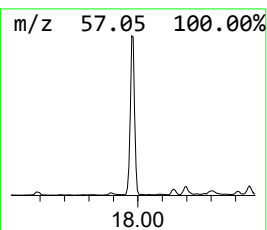
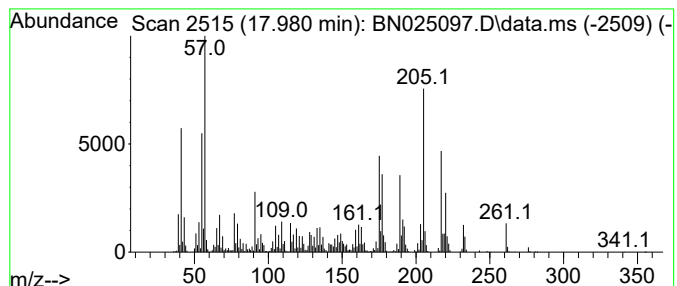
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.980	6.31 ng/ul	1567330	Phenanthrene-d10	17.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99		
2	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	95		
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	83		
4	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	50		
5	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	50		



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042223\
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Sample : 02399-13
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
COMP1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	7.975	2.8	ng/ul	260642	1	7.916	1896420	20.0
Phenol, 2-methoxy-	9.022	5.7	ng/ul	535915	1	7.916	1896420	20.0
1-(2-Thienyl)-1...	10.640	2.2	ng/ul	316265	2	10.728	2885120	20.0
Vanillin	13.487	10.2	ng/ul	2069060	3	14.563	4042750	20.0
7,9-Di-tert-but...	17.980	6.3	ng/ul	1567330	4	17.310	4965100	20.0