

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042223\
 Data File : BN025100.D
 Acq On : 23 Apr 2023 06:02
 Operator : CG/JU
 Sample : 02399-12
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 COMN3

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: BN025100.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	15	18	27	rVB	74855	101256	0.75%	0.087%
2	3.722	90	91	112	rBV	327678	595597	4.38%	0.513%
3	3.958	127	131	135	rVB2	14726	21044	0.15%	0.018%
4	4.052	143	147	156	rVB	28310	44587	0.33%	0.038%
5	4.434	208	212	218	rVB7	9788	16595	0.12%	0.014%
6	5.211	338	344	348	rBV7	7465	14354	0.11%	0.012%
7	5.434	378	382	386	rVB2	18986	29278	0.22%	0.025%
8	5.952	465	470	475	rVB3	15856	23480	0.17%	0.020%
9	6.899	627	631	636	rBV5	11951	20987	0.15%	0.018%
10	7.010	646	650	653	rBV5	15759	27298	0.20%	0.023%
11	7.075	653	661	675	rVB	325990	568958	4.19%	0.490%
12	7.246	683	690	705	rVB	1498143	2369518	17.44%	2.040%
13	7.446	715	724	733	rBV	1300448	2113270	15.56%	1.819%
14	7.916	797	804	810	rBV	1230032	1946650	14.33%	1.676%
15	7.975	810	814	826	rVB	162233	255334	1.88%	0.220%
16	8.205	850	853	860	rVB7	10155	18372	0.14%	0.016%
17	8.534	905	909	914	rVB	27145	40049	0.29%	0.034%
18	8.628	918	925	935	rBV	978952	1592007	11.72%	1.370%
19	8.746	941	945	952	rVB	40402	66088	0.49%	0.057%
20	9.022	983	992	997	rBV	336583	549931	4.05%	0.473%
21	9.087	997	1003	1008	rVV	1876593	3052509	22.47%	2.627%
22	9.134	1008	1011	1017	rVB	65510	107052	0.79%	0.092%
23	9.246	1024	1030	1036	rVB4	32024	57392	0.42%	0.049%
24	9.487	1065	1071	1080	rVB	24197	47881	0.35%	0.041%
25	9.810	1116	1126	1138	rBV	1522288	2496538	18.38%	2.149%
26	10.034	1159	1164	1171	rVB6	18700	34409	0.25%	0.030%
27	10.346	1208	1217	1227	rBV	2013672	3285833	24.19%	2.828%
28	10.499	1240	1243	1250	rVB8	10172	17830	0.13%	0.015%
29	10.587	1253	1258	1260	rBV6	10944	16027	0.12%	0.014%
30	10.634	1260	1266	1274	rVV2	156893	302763	2.23%	0.261%
31	10.728	1274	1282	1288	rVV	1797141	2979583	21.93%	2.565%
32	10.781	1288	1291	1297	rVV	76507	117483	0.86%	0.101%
33	10.869	1298	1306	1319	rVV	2133170	3561587	26.22%	3.066%
34	10.963	1320	1322	1328	rVB6	11425	15365	0.11%	0.013%
35	11.322	1379	1383	1389	rVV7	7682	14402	0.11%	0.012%
36	11.387	1389	1394	1404	rVB2	24981	56483	0.42%	0.049%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoother: OFF

Sampling : 1

Start Thrs: 0.2

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Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.M
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37	11.522	1411	1417	1427	rVB4	58475	116740	0.86%	0.100%
38	11.898	1475	1481	1491	rBV	43773	81026	0.60%	0.070%
39	12.010	1491	1500	1513	rVB	319327	569065	4.19%	0.490%
40	12.316	1544	1552	1560	rVB3	46000	84226	0.62%	0.072%
41	12.622	1598	1604	1612	rVB5	9257	20987	0.15%	0.018%
42	12.769	1624	1629	1635	rVB9	11966	19682	0.14%	0.017%
43	12.863	1635	1645	1649	rBV10	19030	44128	0.32%	0.038%
44	12.916	1649	1654	1658	rBV7	12030	22607	0.17%	0.019%
45	13.163	1691	1696	1701	rBV3	13532	17545	0.13%	0.015%
46	13.487	1741	1751	1765	rBV	1409936	2031995	14.96%	1.749%
47	13.604	1765	1771	1780	rVB2	22503	41275	0.30%	0.036%
48	13.975	1827	1834	1843	rBV	4396909	6031562	44.40%	5.192%
49	14.081	1848	1852	1857	rVB8	7555	13792	0.10%	0.012%
50	14.257	1870	1882	1894	rBV	4847032	7019587	51.68%	6.042%
51	14.345	1894	1897	1904	rVV	19497	30395	0.22%	0.026%
52	14.422	1906	1910	1917	rVB	33295	51898	0.38%	0.045%
53	14.563	1926	1934	1941	rVV	2827701	4125341	30.37%	3.551%
54	14.640	1943	1947	1955	rVB	50080	76705	0.56%	0.066%
55	14.757	1961	1967	1976	rBV	282469	481580	3.55%	0.415%
56	14.975	2000	2004	2009	rVB7	13130	21897	0.16%	0.019%
57	15.234	2043	2048	2056	rBV	97298	144157	1.06%	0.124%
58	15.363	2062	2070	2079	rVB7	21401	58305	0.43%	0.050%
59	15.557	2095	2103	2113	rBV	6176541	8704990	64.08%	7.493%
60	15.675	2116	2123	2135	rVV	2324316	2973454	21.89%	2.559%
61	15.792	2137	2143	2148	rVV2	36004	62805	0.46%	0.054%
62	15.839	2148	2151	2159	rVV10	9790	18378	0.14%	0.016%
63	15.922	2159	2165	2173	rVB	56553	93473	0.69%	0.080%
64	16.128	2195	2200	2206	rBV8	22773	38969	0.29%	0.034%
65	16.339	2232	2236	2240	rVB5	8753	16392	0.12%	0.014%
66	16.904	2328	2332	2336	rVB5	11579	14405	0.11%	0.012%
67	17.310	2395	2401	2411	rVB	3669669	5023350	36.98%	4.324%
68	17.410	2411	2418	2430	rBV2	7077295	9871052	72.67%	8.497%
69	17.592	2445	2449	2453	rVB	17088	22127	0.16%	0.019%
70	17.692	2463	2466	2471	rVB4	10621	17905	0.13%	0.015%
71	17.886	2496	2499	2503	rBV6	12950	16544	0.12%	0.014%
72	17.980	2509	2515	2522	rBV	1171656	1466404	10.80%	1.262%
73	18.151	2539	2544	2547	rBV3	19735	27665	0.20%	0.024%
74	18.198	2547	2552	2557	rBV3	43073	62492	0.46%	0.054%
75	18.280	2561	2566	2568	rBV	23164	34487	0.25%	0.030%
76	18.410	2584	2588	2591	rBV5	16338	19995	0.15%	0.017%

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77	18.457	2592	2596	2601	rVB3	30098	37105	0.27%	0.032%
78	18.704	2634	2638	2641	rBV5	14049	21096	0.16%	0.018%
79	18.786	2649	2652	2657	rBV4	11841	19189	0.14%	0.017%
80	19.269	2729	2734	2740	rBV2	95404	130020	0.96%	0.112%
81	19.333	2740	2745	2751	rBV	90050	145050	1.07%	0.125%
82	19.475	2765	2769	2772	rBV2	34772	49071	0.36%	0.042%
83	19.622	2791	2794	2800	rVB2	36106	42667	0.31%	0.037%
84	19.704	2802	2808	2814	rBV	8774632	11706822	86.18%	10.077%
85	19.933	2844	2847	2852	rVB6	26497	35602	0.26%	0.031%
86	20.669	2970	2972	2974	rBV3	28378	26749	0.20%	0.023%
87	20.704	2975	2978	2981	rBV2	81526	92132	0.68%	0.079%
88	21.498	3107	3113	3123	rBV	4513786	5987780	44.08%	5.154%
89	22.604	3297	3301	3306	rBV2	255481	353491	2.60%	0.304%
90	23.163	3392	3396	3405	rVB	202135	308902	2.27%	0.266%
91	23.768	3490	3499	3514	rBV2	6604867	13583985	100.00%	11.692%
92	23.921	3518	3525	3536	rVB	3189133	6330543	46.60%	5.449%
93	24.521	3622	3627	3637	rVB	270823	555256	4.09%	0.478%
94	25.362	3766	3770	3780	rVB2	261259	584571	4.30%	0.503%

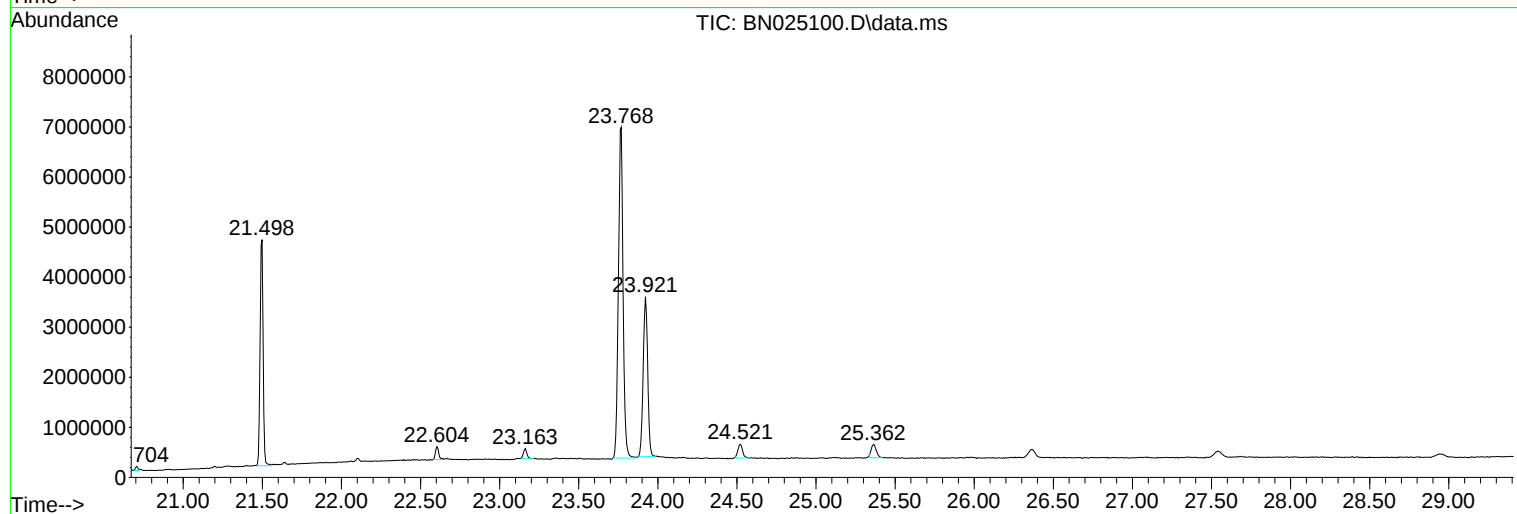
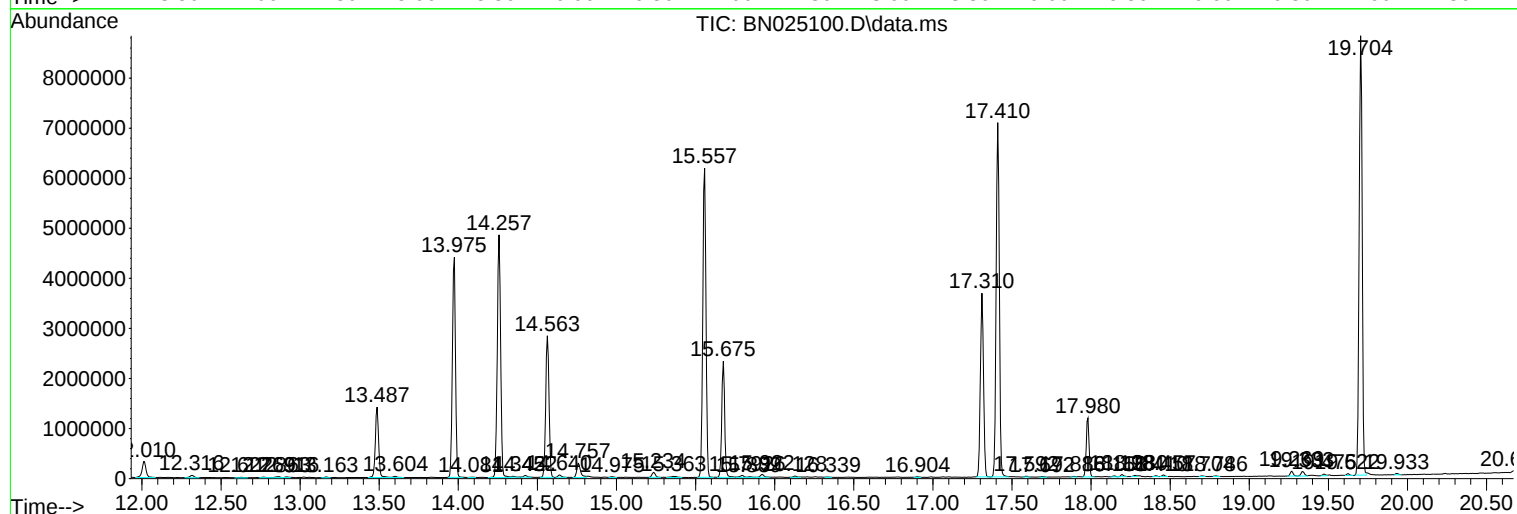
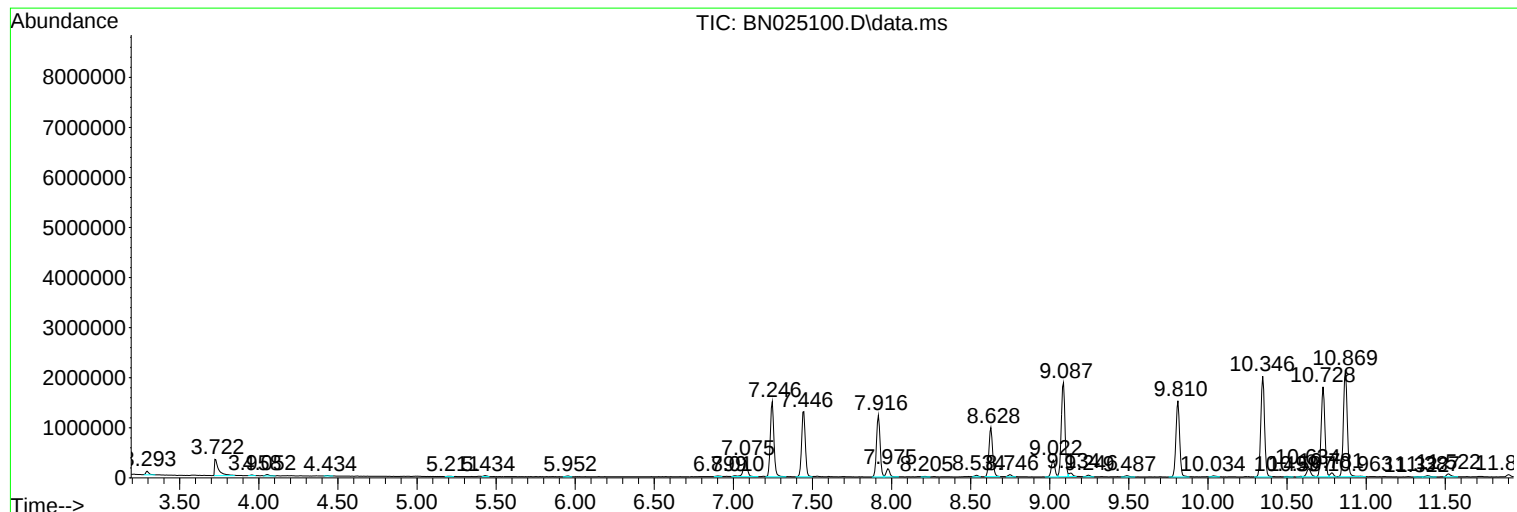
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.M
Quant Title : SVOA CALIBRATION

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



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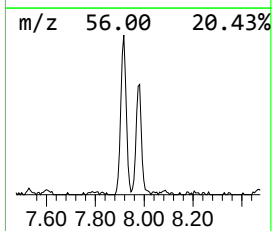
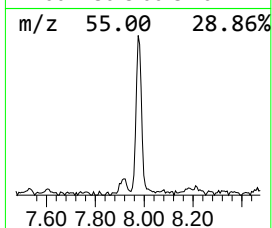
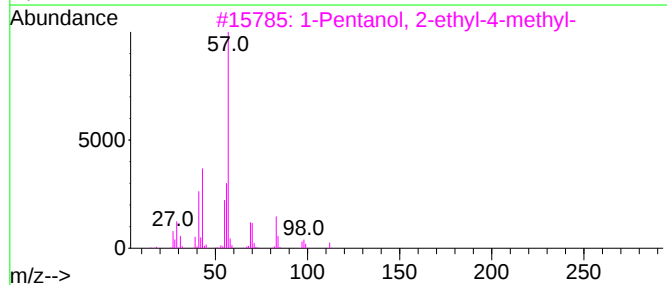
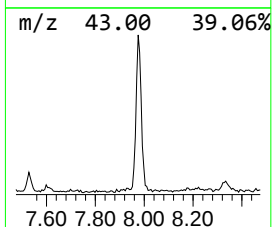
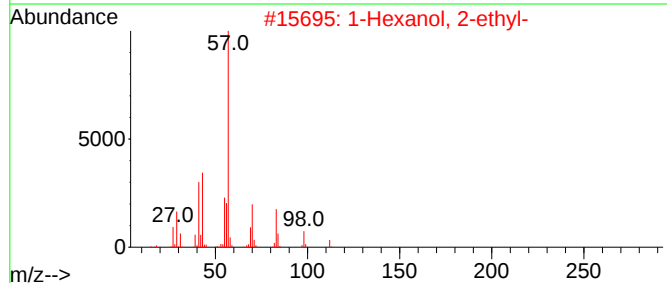
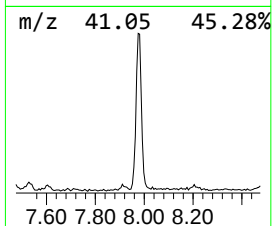
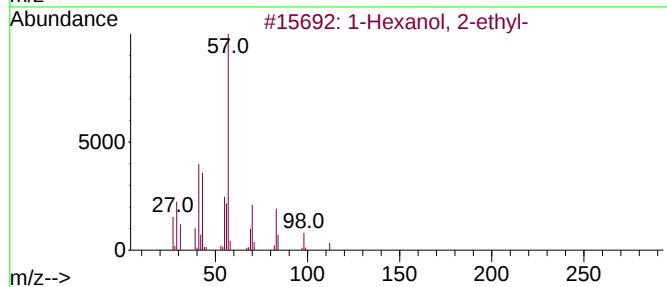
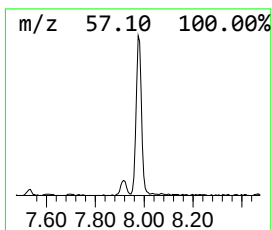
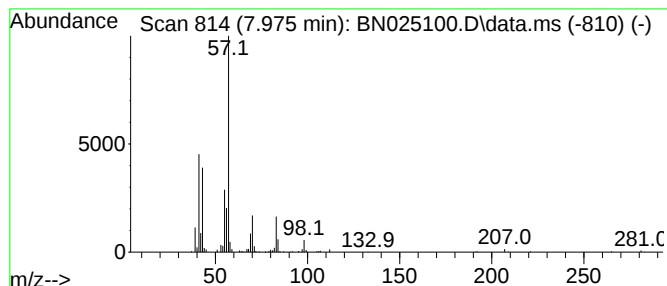
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.M
Quant Title : SVOA CALIBRATION

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	2.62 ng/ul	255334	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	72
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
3	1-Pentanol, 2-ethyl-4-methyl-			130	C8H18O	000106-67-2	56
4	Carbonic acid, heptyl vinyl ester			186	C10H18O3	1010383-25-4	53
5	Heptyl isobutyl carbonate			216	C12H24O3	959068-08-7	53



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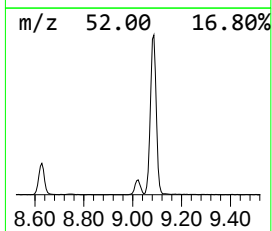
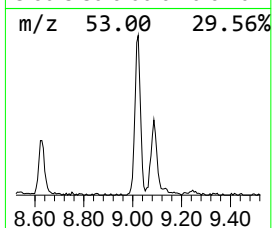
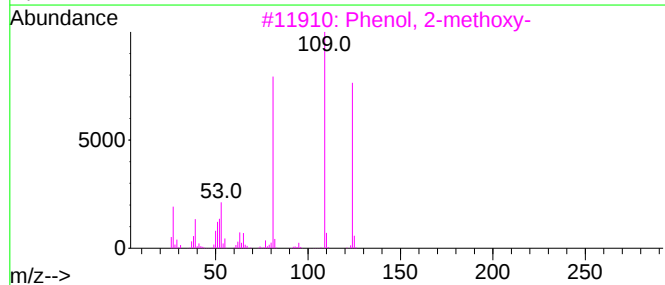
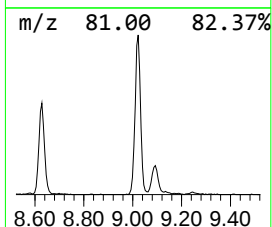
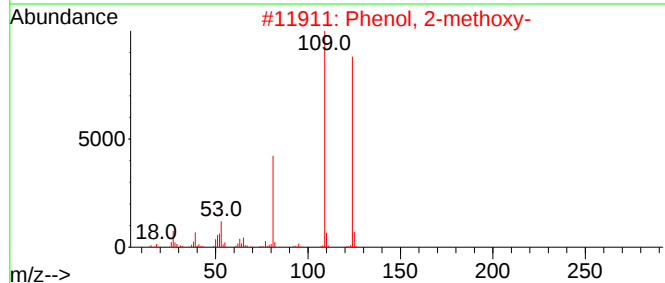
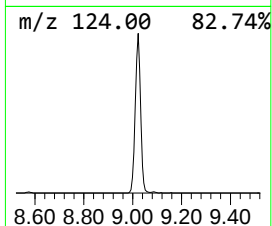
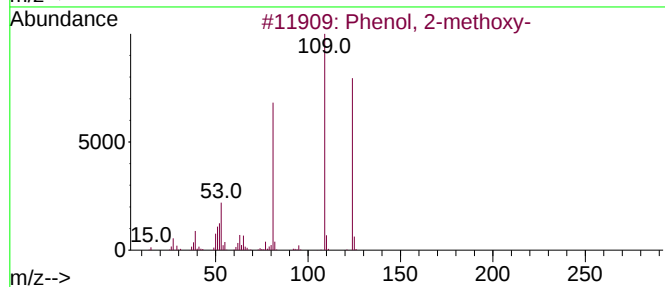
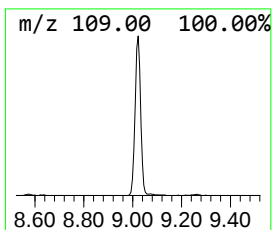
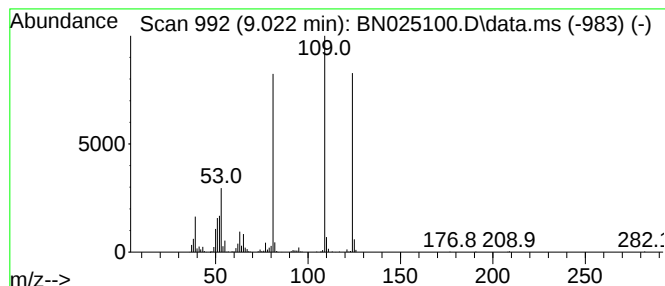
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.M
Quant Title : SVOA CALIBRATION

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	549931	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	93
3			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	93
4			Mequinol	124	C7H8O2	000150-76-5	90
5			Mequinol	124	C7H8O2	000150-76-5	90



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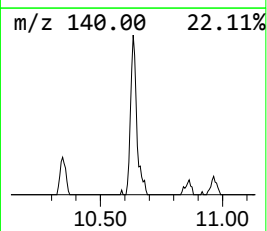
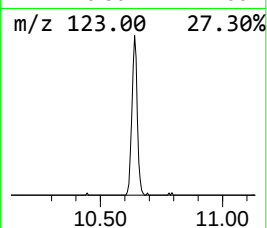
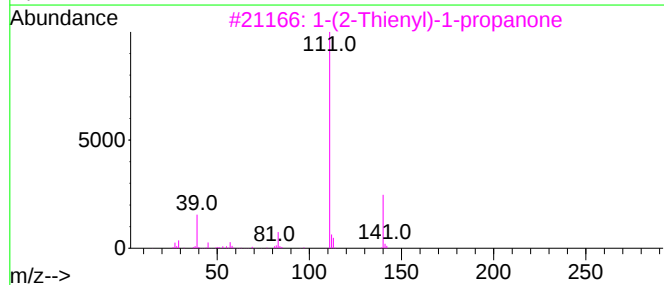
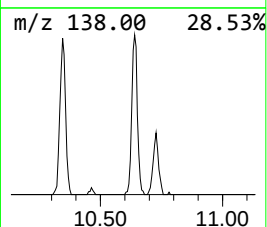
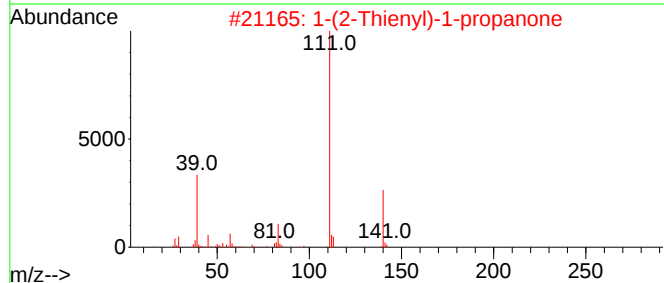
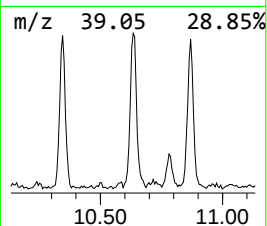
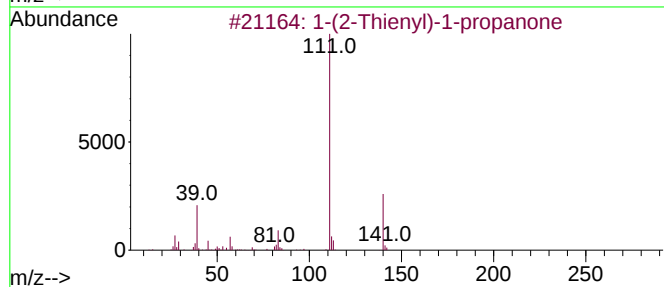
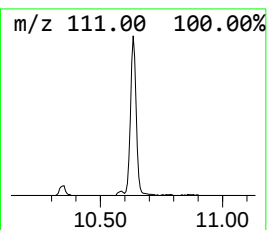
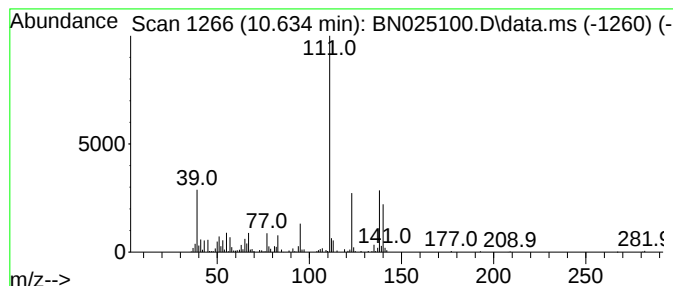
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.634	2.03 ng/ul	302763	Naphthalene-d8	10.728

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-(2-Thienyl)-1-propanone	140	C7H8OS	013679-75-9	64
2			1-(2-Thienyl)-1-propanone	140	C7H8OS	013679-75-9	64
3			1-(2-Thienyl)-1-propanone	140	C7H8OS	013679-75-9	52
4			Glycine, N-(2-thienylcarbonyl)-,...	199	C8H9NO3S	1000299-60-2	50
5			2H-Pyran-2-carboxaldehyde, 3,4-d...	140	C8H12O2	001920-21-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042223\
Data File : BN025100.D
Acq On : 23 Apr 2023 06:02
Operator : CG/JU
Sample : 02399-12
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
COMN3

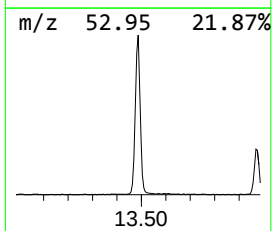
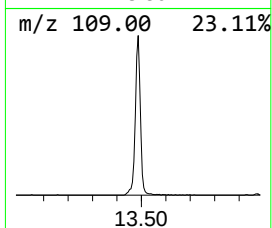
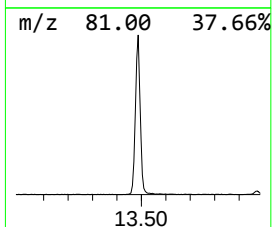
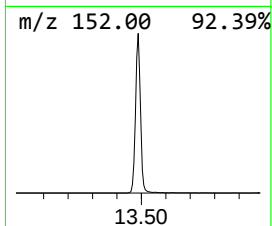
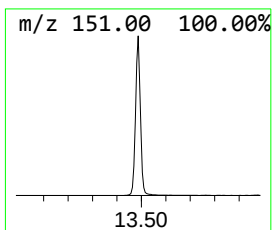
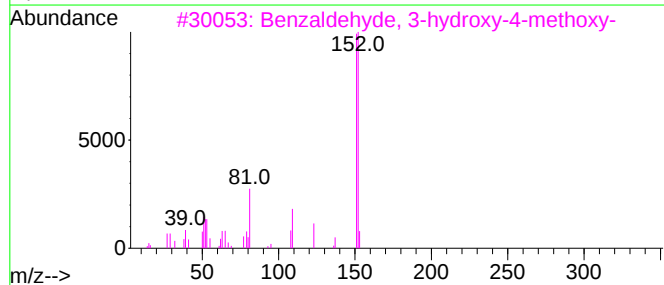
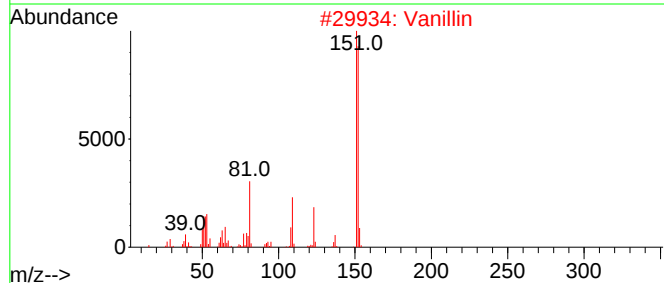
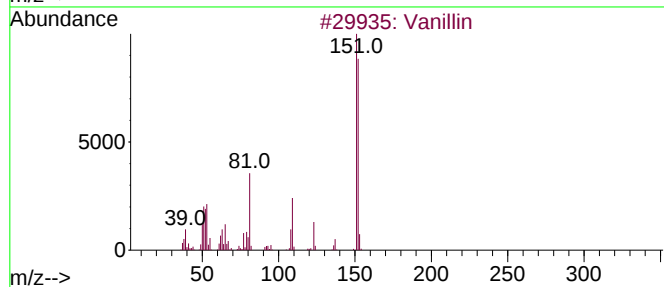
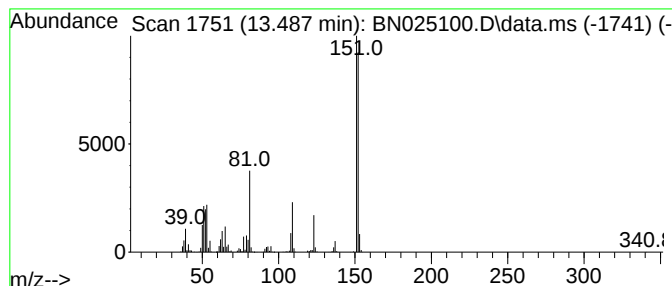
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Quant Title : SVOA CALIBRATION

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	9.85 ng/ul	2032000	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			Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	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 : BN025100.D
Acq On : 23 Apr 2023 06:02
Operator : CG/JU
Sample : 02399-12
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
COMN3

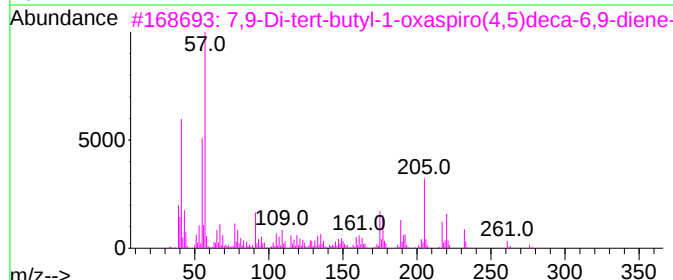
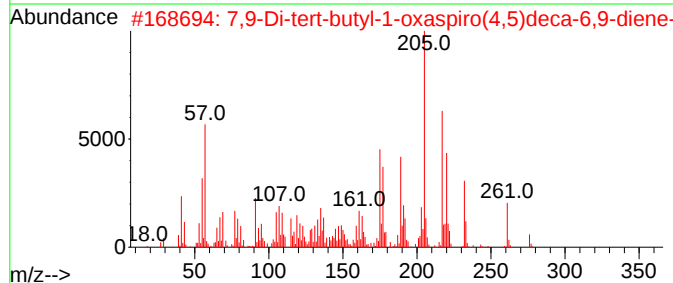
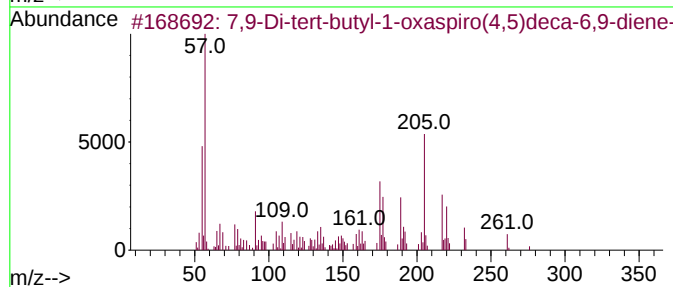
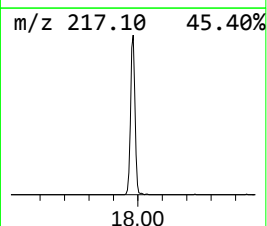
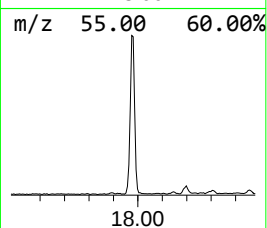
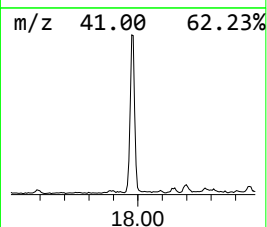
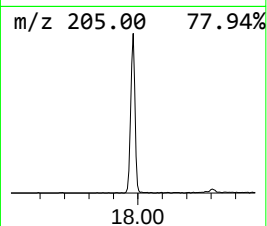
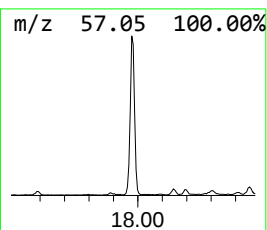
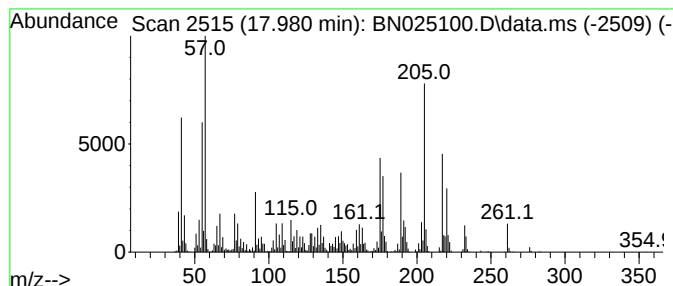
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.M
Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.980	5.84 ng/ul	1466400	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	89		
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	60		
4	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	50		
5	Ethanone, 1-(5,6,7,8-tetrahydro...	220	C14H20O2	071596-88-8	45		



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042223\
Data File : BN025100.D
Acq On : 23 Apr 2023 06:02
Operator : CG/JU
Sample : 02399-12
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
COMN3

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	2.6	ng/ul	255334	1	7.916	1946650	20.0
Phenol, 2-methoxy-	9.022	5.7	ng/ul	549931	1	7.916	1946650	20.0
1-(2-Thienyl)-1...	10.634	2.0	ng/ul	302763	2	10.728	2979580	20.0
Vanillin	13.487	9.8	ng/ul	2032000	3	14.563	4125340	20.0
7,9-Di-tert-but...	17.980	5.8	ng/ul	1466400	4	17.310	5023350	20.0