

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042223\
 Data File : BN025077.D
 Acq On : 22 Apr 2023 15:44
 Operator : CG/JU
 Sample : 02399-05
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 COMM3

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: BN025077.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	24	rBV	51442	69281	0.72%	0.087%
2	3.734	92	93	106	rBV	89116	183160	1.90%	0.229%
3	3.958	127	131	139	rVB9	11272	22771	0.24%	0.029%
4	4.058	143	148	153	rVV	18030	26683	0.28%	0.033%
5	4.428	207	211	216	rBV7	10739	15173	0.16%	0.019%
6	5.434	379	382	390	rVB	13804	21811	0.23%	0.027%
7	5.952	466	470	477	rVB6	11160	22630	0.23%	0.028%
8	6.899	625	631	636	rBV8	11946	22615	0.23%	0.028%
9	7.011	646	650	653	rBV4	9759	15272	0.16%	0.019%
10	7.075	653	661	670	rVB	255328	437800	4.54%	0.548%
11	7.246	683	690	704	rVB	1099346	1709928	17.72%	2.142%
12	7.446	715	724	734	rBV	960711	1545413	16.01%	1.936%
13	7.916	794	804	810	rBV	913729	1449622	15.02%	1.816%
14	7.981	810	815	827	rVB	110546	184602	1.91%	0.231%
15	8.210	851	854	860	rVB7	8260	13859	0.14%	0.017%
16	8.540	905	910	915	rBV2	17883	30806	0.32%	0.039%
17	8.628	918	925	935	rVV	742872	1191263	12.34%	1.492%
18	8.746	941	945	952	rVB	28238	46183	0.48%	0.058%
19	9.022	986	992	997	rBV	231315	374144	3.88%	0.469%
20	9.087	997	1003	1009	rVV	1348485	2178309	22.57%	2.728%
21	9.134	1009	1011	1020	rVB	49001	72330	0.75%	0.091%
22	9.246	1025	1030	1037	rVB8	21261	38994	0.40%	0.049%
23	9.487	1067	1071	1078	rVB2	17753	29675	0.31%	0.037%
24	9.810	1117	1126	1138	rBV	1065920	1725709	17.88%	2.161%
25	10.040	1160	1165	1172	rBV6	15993	29439	0.31%	0.037%
26	10.246	1195	1200	1205	rBV9	6753	13697	0.14%	0.017%
27	10.346	1210	1217	1229	rBV	1374077	2249212	23.30%	2.817%
28	10.499	1241	1243	1250	rVB6	7024	11058	0.11%	0.014%
29	10.593	1253	1259	1260	rBV6	8876	16796	0.17%	0.021%
30	10.640	1260	1267	1275	rVV2	106275	199572	2.07%	0.250%
31	10.728	1275	1282	1288	rVV	1240884	2026716	21.00%	2.538%
32	10.787	1288	1292	1298	rVB	46878	75347	0.78%	0.094%
33	10.869	1298	1306	1319	rBV	977298	1666431	17.27%	2.087%
34	11.393	1390	1395	1403	rVB3	16149	33107	0.34%	0.041%
35	11.516	1411	1416	1428	rBV5	43196	88716	0.92%	0.111%
36	11.904	1476	1482	1488	rBV	32345	50045	0.52%	0.063%

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Integrator: RTE

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Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	12.016	1492	1501	1515	rVB	207466	377909	3.92%	0.473%
38	12.316	1544	1552	1559	rVB3	29031	53508	0.55%	0.067%
39	12.775	1621	1630	1635	rBV3	10253	19909	0.21%	0.025%
40	12.840	1635	1641	1649	rVV3	6381	19352	0.20%	0.024%
41	12.922	1649	1655	1663	rVB8	12373	30223	0.31%	0.038%
42	13.022	1668	1672	1677	rVB5	7215	10083	0.10%	0.013%
43	13.163	1693	1696	1703	rBV9	8658	15171	0.16%	0.019%
44	13.487	1740	1751	1765	rBV	1054301	1512174	15.67%	1.894%
45	13.598	1765	1770	1782	rVB4	32352	57884	0.60%	0.072%
46	13.975	1827	1834	1844	rVB	3156600	4253352	44.07%	5.327%
47	14.257	1875	1882	1894	rVV	3283586	4645646	48.13%	5.818%
48	14.351	1894	1898	1902	rVV2	15112	25900	0.27%	0.032%
49	14.428	1906	1911	1917	rVB	28404	49164	0.51%	0.062%
50	14.563	1926	1934	1942	rBV	2060422	2951809	30.58%	3.697%
51	14.640	1943	1947	1953	rVV2	33855	48535	0.50%	0.061%
52	14.763	1960	1968	1976	rBV	215273	375022	3.89%	0.470%
53	14.822	1976	1978	1984	rVB3	15270	21243	0.22%	0.027%
54	14.975	1999	2004	2010	rVB9	12485	21791	0.23%	0.027%
55	15.234	2042	2048	2055	rBV	75622	117678	1.22%	0.147%
56	15.369	2063	2071	2077	rBV10	16165	43538	0.45%	0.055%
57	15.557	2096	2103	2109	rBV	4234933	5954460	61.70%	7.458%
58	15.675	2117	2123	2132	rBV	1622625	2088079	21.64%	2.615%
59	15.798	2137	2144	2148	rVB3	21516	36561	0.38%	0.046%
60	15.922	2161	2165	2169	rBV	43614	61618	0.64%	0.077%
61	16.134	2194	2201	2205	rBV7	18574	36162	0.37%	0.045%
62	16.334	2233	2235	2241	rVB7	7463	12916	0.13%	0.016%
63	17.269	2390	2394	2395	rBV4	7837	10365	0.11%	0.013%
64	17.310	2395	2401	2410	rVV	2560775	3592367	37.22%	4.499%
65	17.410	2412	2418	2431	rVV2	4825282	6810169	70.56%	8.529%
66	17.592	2445	2449	2453	rBV3	13678	18761	0.19%	0.023%
67	17.981	2509	2515	2520	rBV	810471	990869	10.27%	1.241%
68	18.151	2541	2544	2547	rVB3	13976	16074	0.17%	0.020%
69	18.198	2547	2552	2560	rBV	77587	121722	1.26%	0.152%
70	18.281	2563	2566	2568	rBV	19273	22790	0.24%	0.029%
71	18.410	2586	2588	2593	rVV4	13160	13273	0.14%	0.017%
72	18.457	2593	2596	2600	rVB3	21109	27961	0.29%	0.035%
73	18.704	2634	2638	2646	rBV10	10027	16292	0.17%	0.020%
74	19.269	2730	2734	2741	rBV2	58651	83097	0.86%	0.104%
75	19.339	2741	2746	2752	rBV	62312	104106	1.08%	0.130%
76	19.475	2765	2769	2773	rBV3	68376	86311	0.89%	0.108%

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 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

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77	19.628	2792	2795	2798	rBV4	19482	24112	0.25%	0.030%
78	19.704	2802	2808	2815	rBV	5999271	8181570	84.77%	10.247%
79	19.939	2845	2848	2853	rVB5	23936	27044	0.28%	0.034%
80	20.710	2977	2979	2982	rBV2	26294	30592	0.32%	0.038%
81	21.504	3109	3114	3124	rBV2	3204317	4341783	44.99%	5.438%
82	23.798	3496	3504	3519	rBV2	4527648	9651325	100.00%	12.088%
83	23.951	3523	3530	3543	rVB2	2631774	4944261	51.23%	6.193%

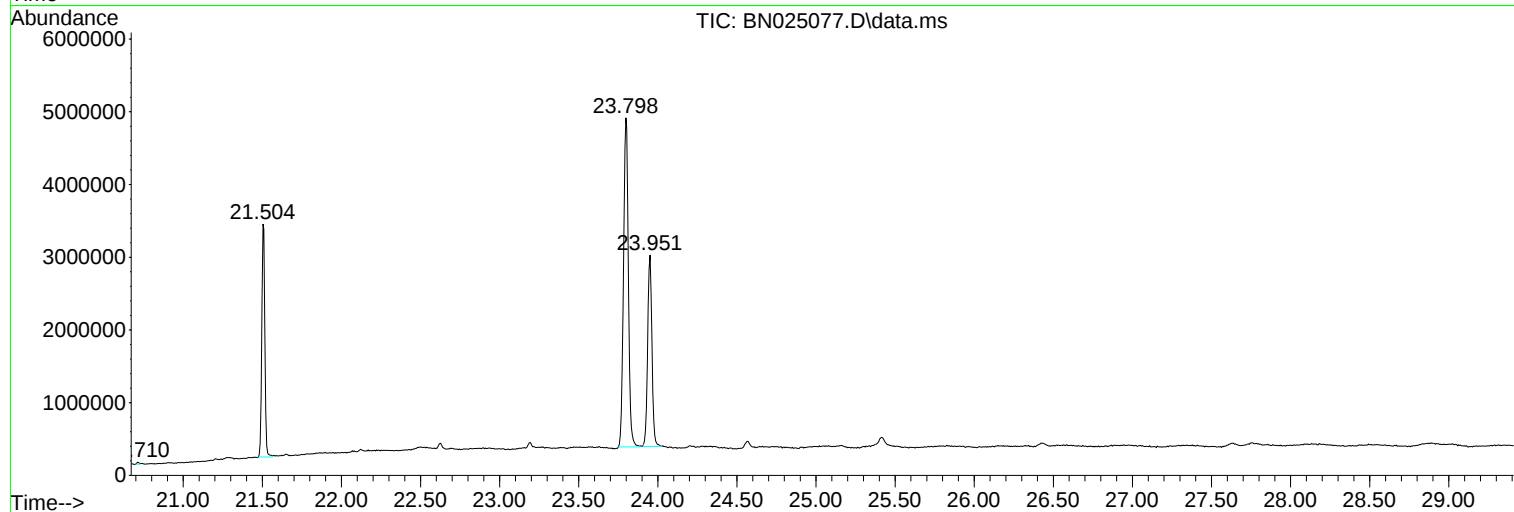
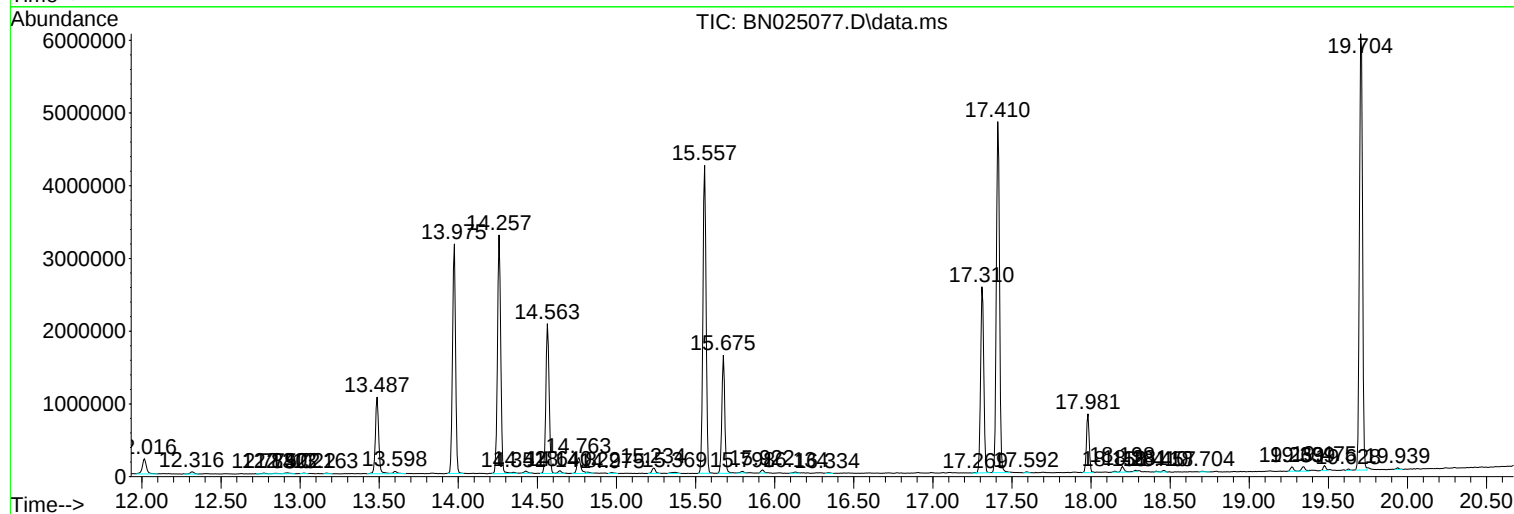
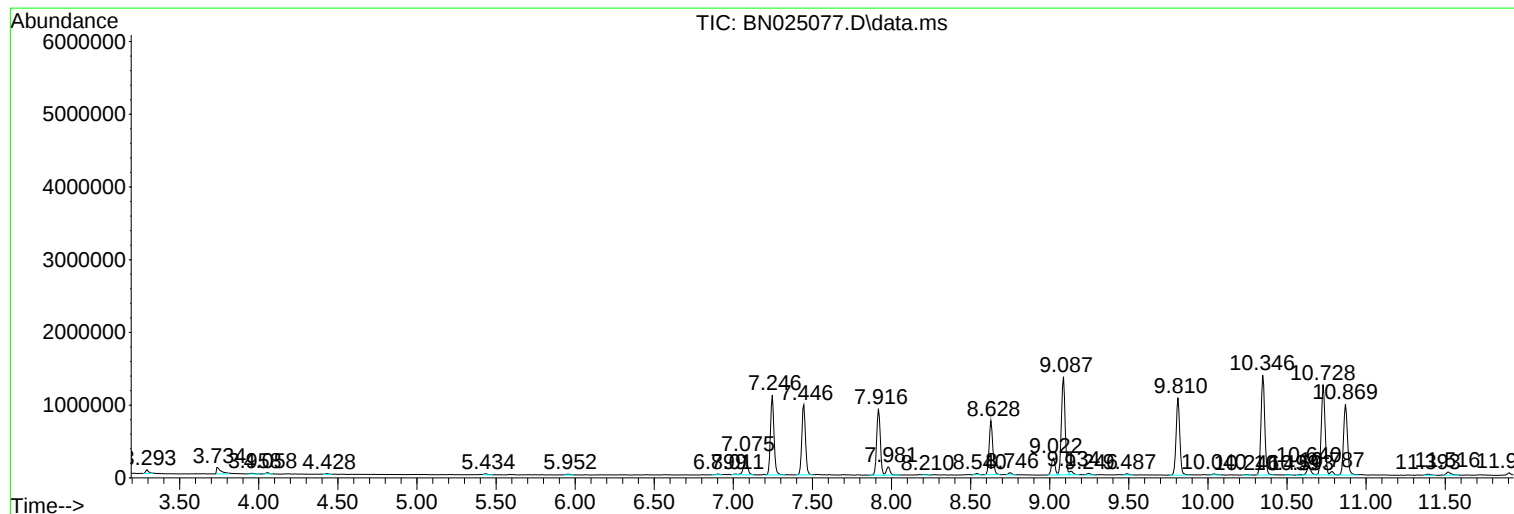
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.M
Quant Title : SVOA CALIBRATION

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



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Sample : 02399-05
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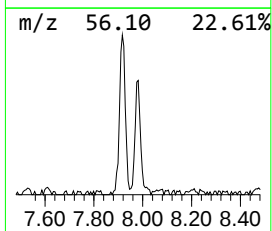
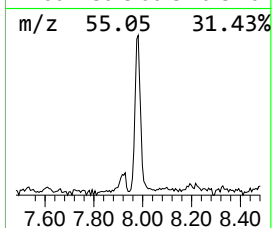
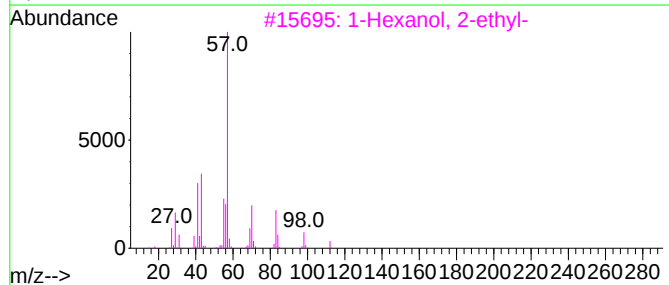
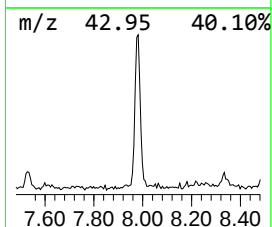
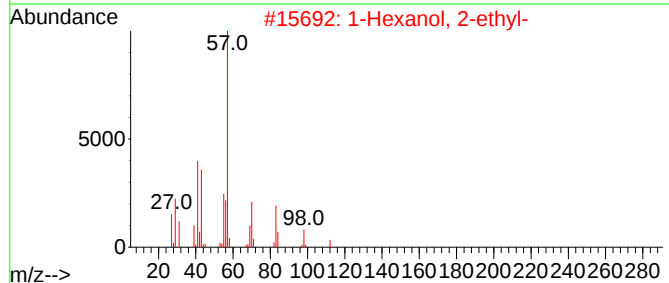
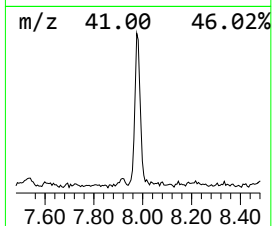
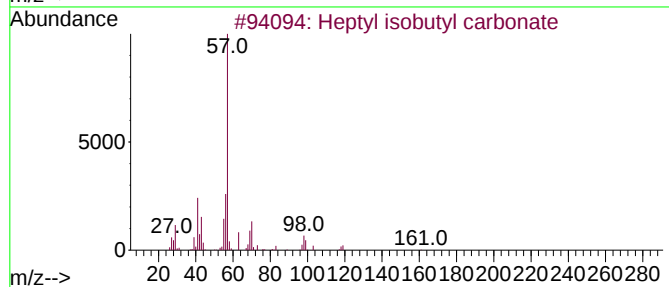
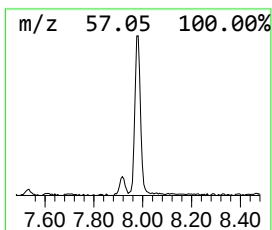
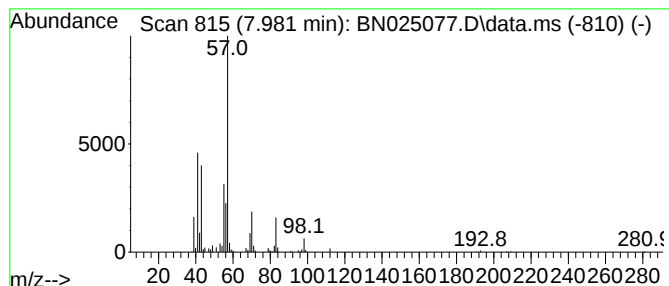
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Heptyl isobutyl carbonate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.981	2.55 ng/ul	184602	1,4-Dichlorobenzene-d4	7.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	64
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	50
4			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	50
5			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	45



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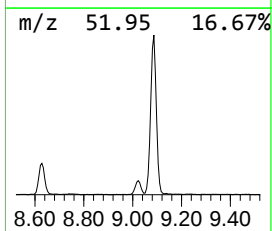
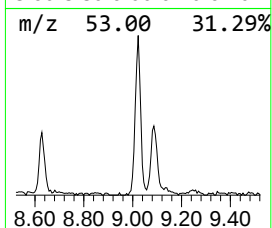
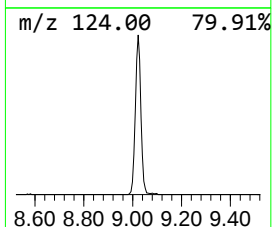
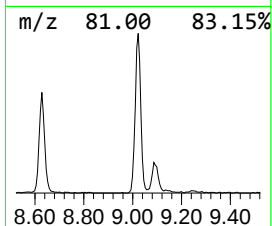
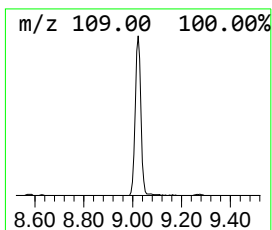
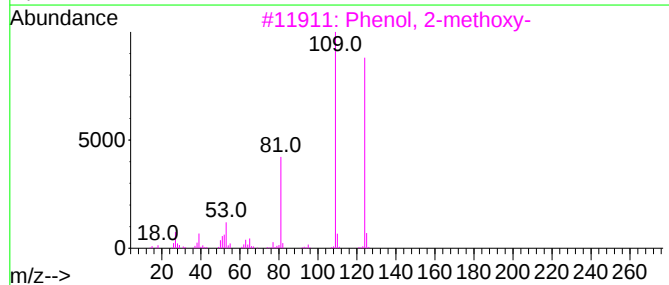
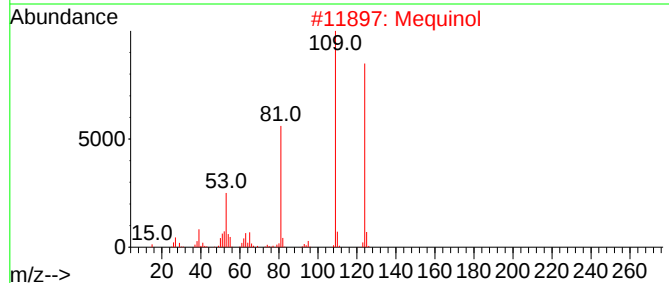
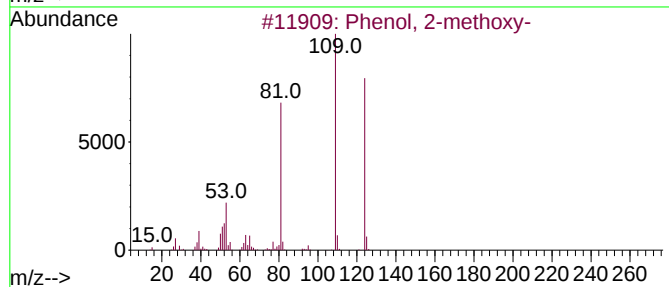
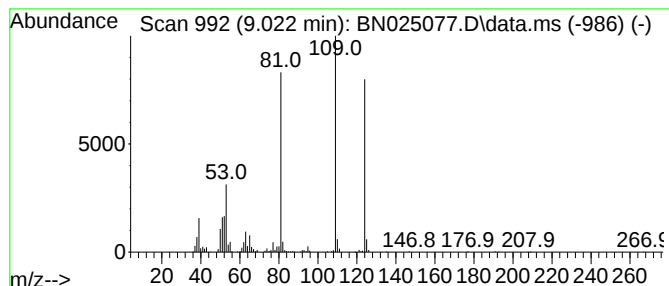
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.M
Quant Title : SVOA CALIBRATION

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	5.16 ng/ul	374144	1,4-Dichlorobenzene-d4	7.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	95
2			Mequinol	124	C7H8O2	000150-76-5	92
3			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	91
4			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	90
5			Mequinol	124	C7H8O2	000150-76-5	90



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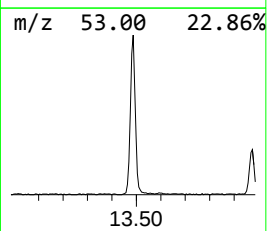
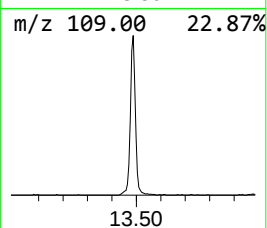
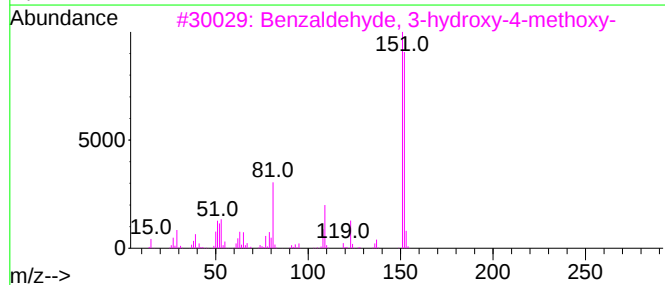
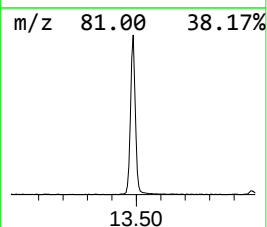
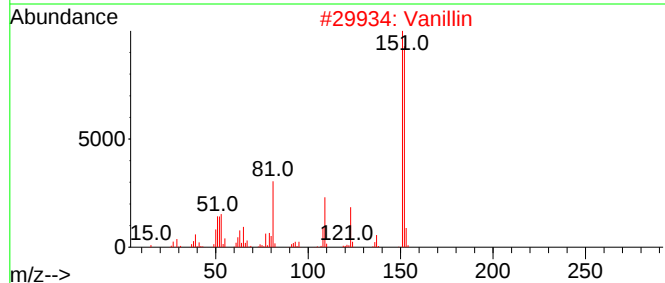
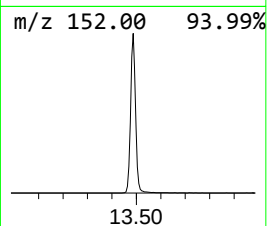
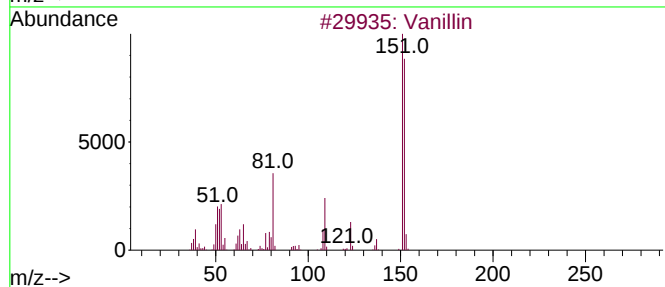
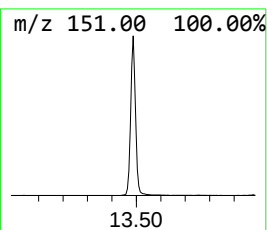
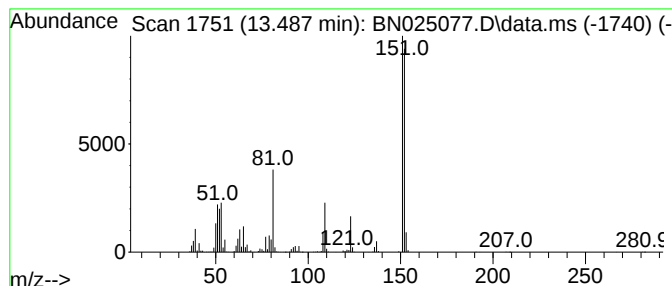
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Vanillin Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.487	10.25 ng/ul	1512170	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



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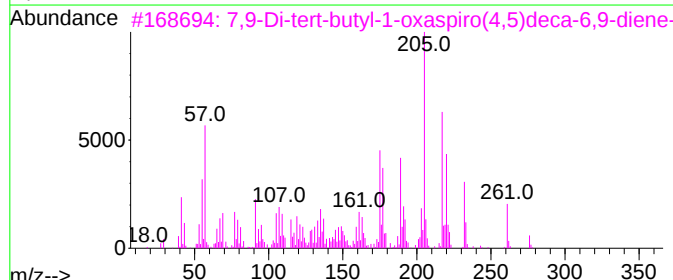
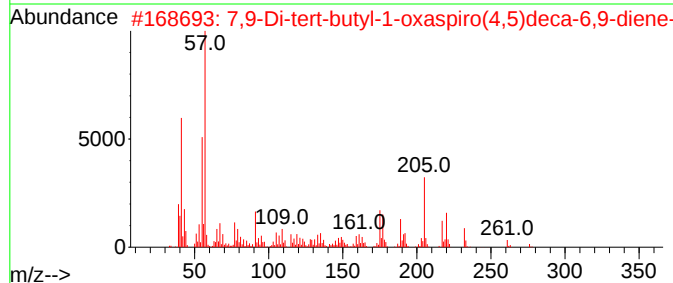
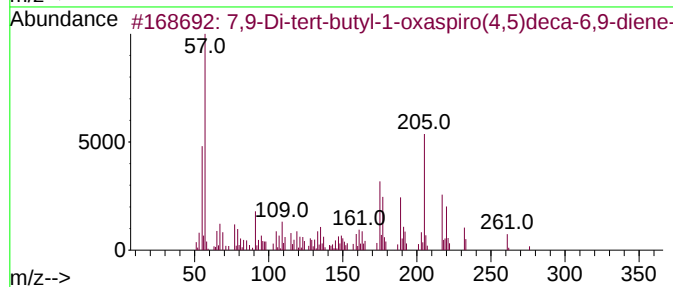
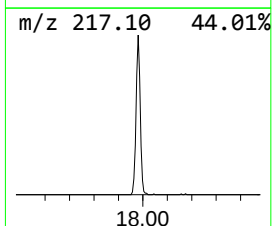
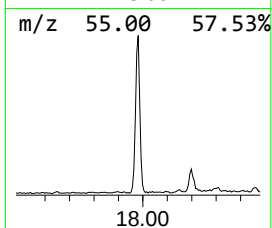
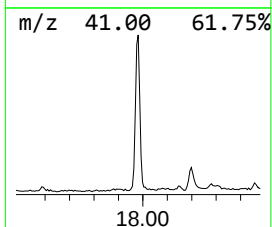
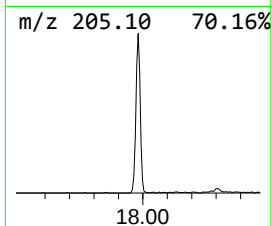
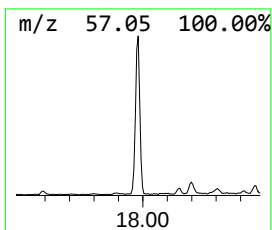
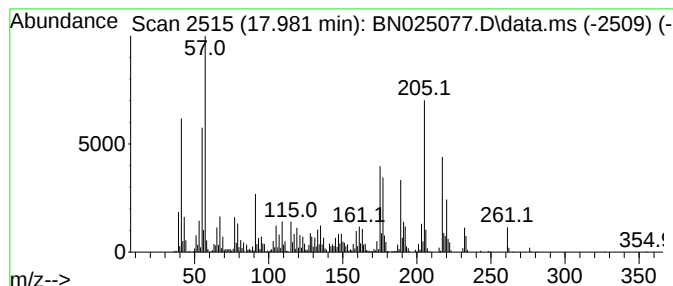
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.981	5.52 ng/ul	990869	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	70		
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	50		
4	2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	48		
5	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	42		



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042223\
Data File : BN025077.D
Acq On : 22 Apr 2023 15:44
Operator : CG/JU
Sample : 02399-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
COMM3

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Heptyl isobutyl...	7.981	2.5	ng/u1	184602	1	7.916	1449620	20.0
Phenol, 2-methoxy-	9.022	5.2	ng/u1	374144	1	7.916	1449620	20.0
Vanillin	13.487	10.3	ng/u1	1512170	3	14.563	2951810	20.0
7,9-Di-tert-but...	17.981	5.5	ng/u1	990869	4	17.310	3592370	20.0