

Data Path : Z:\svoasrv\HPCHEM1\BNA\_N\Data\BN041324\  
 Data File : BN030884.D  
 Acq On : 13 Apr 2024 17:26  
 Operator : MA/JU  
 Sample : P2050-05  
 Misc :  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 BNA\_N  
 ClientSampleId :  
 MCOR79

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-BN032824.MA.M  
 Title : SVOA CALIBRATION

Signal : TIC: BN030884.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.175	28	32	40	rBV	23872	36978	0.55%	0.073%
2	3.587	99	102	123	rBV	106325	209474	3.11%	0.416%
3	3.899	152	155	158	rBV	6769	7211	0.11%	0.014%
4	5.234	378	382	388	rVB2	8226	12521	0.19%	0.025%
5	5.740	463	468	471	rBV6	6827	11825	0.18%	0.023%
6	6.781	640	645	646	rBV3	7274	10643	0.16%	0.021%
7	6.834	646	654	665	rVB	131702	239692	3.56%	0.476%
8	7.005	677	683	695	rVB	625902	982113	14.58%	1.949%
9	7.199	708	716	727	rBV	562079	879099	13.05%	1.745%
10	7.281	727	730	739	rVB10	4764	11587	0.17%	0.023%
11	7.663	788	795	801	rBV	474233	751725	11.16%	1.492%
12	7.728	801	806	816	rVB	92852	146908	2.18%	0.292%
13	7.946	840	843	847	rVB6	5427	7761	0.12%	0.015%
14	8.210	884	888	892	rBV6	4920	8402	0.12%	0.017%
15	8.281	894	900	904	rVV2	15812	27453	0.41%	0.054%
16	8.369	908	915	927	rVV	430759	706186	10.48%	1.402%
17	8.487	930	935	944	rVB	20183	36960	0.55%	0.073%
18	8.757	974	981	986	rBV	183634	298525	4.43%	0.593%
19	8.822	986	992	997	rVV	739429	1209297	17.95%	2.400%
20	8.863	997	999	1008	rVB	37870	61335	0.91%	0.122%
21	8.981	1013	1019	1024	rVB7	9493	17474	0.26%	0.035%
22	9.216	1052	1059	1065	rVB2	10324	18644	0.28%	0.037%
23	9.534	1104	1113	1129	rBV	531092	878420	13.04%	1.743%
24	9.763	1147	1152	1158	rVB7	5403	11346	0.17%	0.023%
25	9.969	1179	1187	1192	rVB8	6130	15805	0.23%	0.031%
26	10.069	1196	1204	1215	rBV	855001	1403253	20.83%	2.785%
27	10.228	1228	1231	1238	rVB8	5054	7682	0.11%	0.015%
28	10.357	1248	1253	1261	rBV	76498	133231	1.98%	0.264%
29	10.446	1261	1268	1275	rVV	701010	1151261	17.09%	2.285%
30	10.504	1275	1278	1284	rVB	28853	43896	0.65%	0.087%
31	10.587	1285	1292	1304	rBV	807957	1388535	20.61%	2.756%
32	11.104	1374	1380	1384	rVB	16013	27992	0.42%	0.056%
33	11.234	1397	1402	1409	rBV9	9881	18394	0.27%	0.037%
34	11.434	1431	1436	1440	rBV8	4864	9187	0.14%	0.018%
35	11.616	1461	1467	1472	rBV	16280	28141	0.42%	0.056%
36	11.740	1479	1488	1498	rBV	102205	182729	2.71%	0.363%

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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 >  
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37	12.040	1533	1539	1547	rVB3	18482	33677	0.50%	0.067%
38	12.363	1588	1594	1600	rBV8	4338	9113	0.14%	0.018%
39	12.763	1656	1662	1667	rBV4	4925	8214	0.12%	0.016%
40	12.910	1682	1687	1691	rBV4	7872	10513	0.16%	0.021%
41	13.228	1730	1741	1752	rBV	543105	811079	12.04%	1.610%
42	13.345	1757	1761	1767	rVB2	17806	27479	0.41%	0.055%
43	13.722	1819	1825	1839	rBV	1771825	2514054	37.31%	4.990%
44	13.998	1861	1872	1879	rBV	1995659	3023905	44.88%	6.002%
45	14.057	1879	1882	1886	rVV4	14070	22342	0.33%	0.044%
46	14.098	1886	1889	1894	rVV3	8842	15155	0.22%	0.030%
47	14.169	1894	1901	1907	rVB2	26782	50438	0.75%	0.100%
48	14.310	1918	1925	1933	rBV	1122486	1632641	24.23%	3.240%
49	14.392	1935	1939	1945	rVB4	17167	23550	0.35%	0.047%
50	14.516	1954	1960	1968	rBV	100488	191355	2.84%	0.380%
51	14.992	2036	2041	2050	rBV	36845	57877	0.86%	0.115%
52	15.116	2056	2062	2063	rBV3	10317	11936	0.18%	0.024%
53	15.304	2087	2094	2108	rBV	2811844	3935084	58.40%	7.810%
54	15.422	2108	2114	2125	rBV	593896	869012	12.90%	1.725%
55	15.545	2131	2135	2139	rVB5	15801	21145	0.31%	0.042%
56	15.675	2153	2157	2162	rBV	25656	36360	0.54%	0.072%
57	15.881	2185	2192	2198	rBV10	12802	23741	0.35%	0.047%
58	16.092	2223	2228	2232	rVB4	11133	17119	0.25%	0.034%
59	17.057	2386	2392	2402	rVB	1490538	2064842	30.64%	4.098%
60	17.157	2402	2409	2424	rBV2	3282113	4586650	68.07%	9.104%
61	17.351	2438	2442	2449	rVB	21334	28709	0.43%	0.057%
62	17.733	2501	2507	2514	rBV	544773	685463	10.17%	1.361%
63	17.898	2532	2535	2539	rBV6	9619	13092	0.19%	0.026%
64	17.957	2540	2545	2552	rVV2	39703	62973	0.93%	0.125%
65	18.033	2555	2558	2567	rVB	15108	28706	0.43%	0.057%
66	18.169	2577	2581	2584	rBV2	17955	24037	0.36%	0.048%
67	18.210	2585	2588	2592	rVB5	11729	14493	0.22%	0.029%
68	19.022	2721	2726	2733	rBV2	44302	60956	0.90%	0.121%
69	19.092	2734	2738	2742	rBV	35162	49107	0.73%	0.097%
70	19.245	2760	2764	2772	rBV5	32890	56619	0.84%	0.112%
71	19.398	2788	2790	2793	rBV4	7219	6797	0.10%	0.013%
72	19.457	2794	2800	2808	rBV2	4194837	5758053	85.45%	11.429%
73	19.698	2838	2841	2846	rVB7	15275	19172	0.28%	0.038%
74	20.474	2970	2973	2977	rBV3	41267	46031	0.68%	0.091%
75	21.292	3107	3112	3125	rBV	1866554	2703425	40.12%	5.366%
76	24.021	3566	3576	3595	rBV3	2754216	6738249	100.00%	13.374%

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Integration Parameters: LSCINT.P  
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Title : SVOA CALIBRATION

77 24.215 3601 3609 3627 rVB 1265786 3097987 45.98% 6.149%

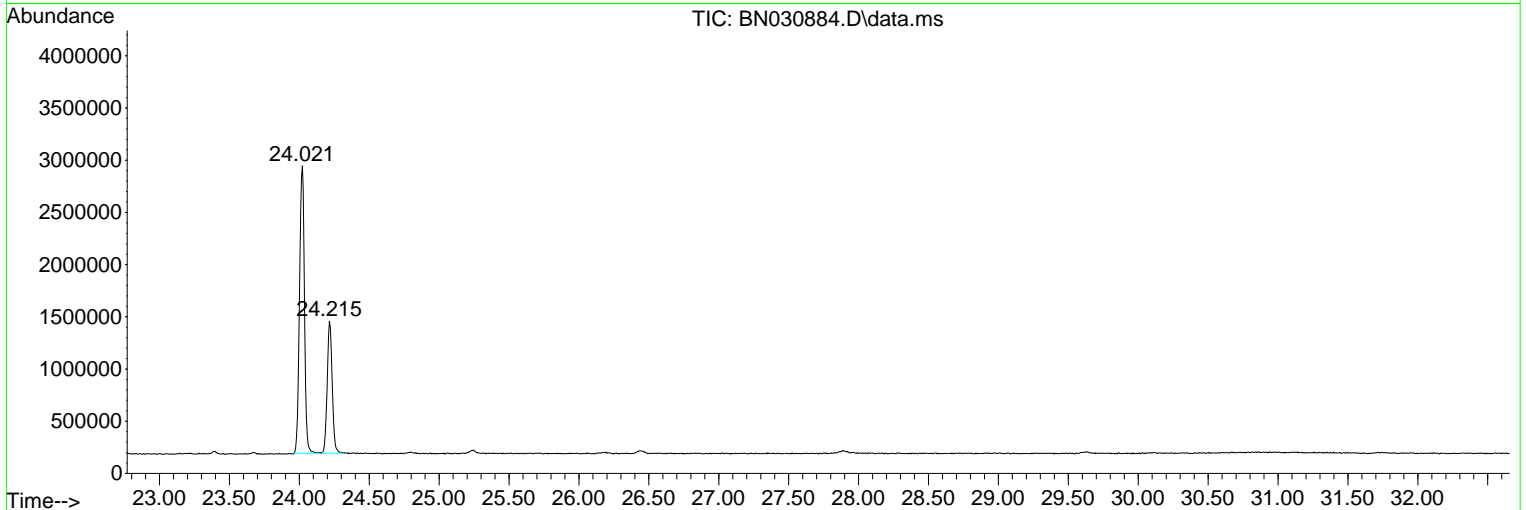
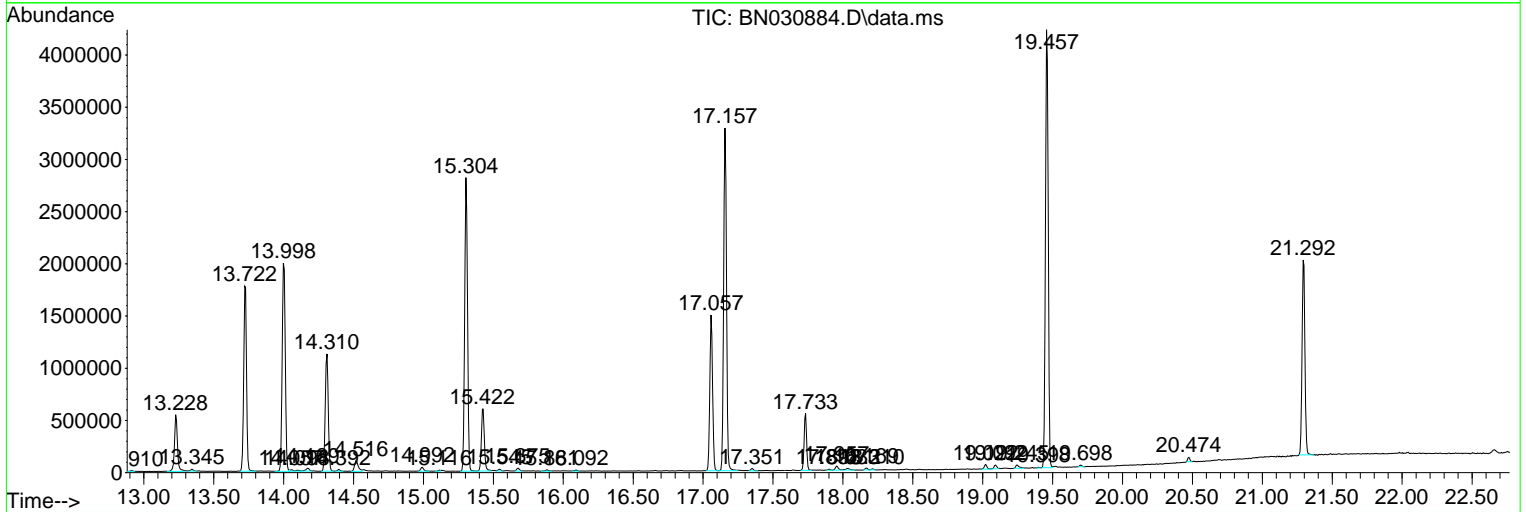
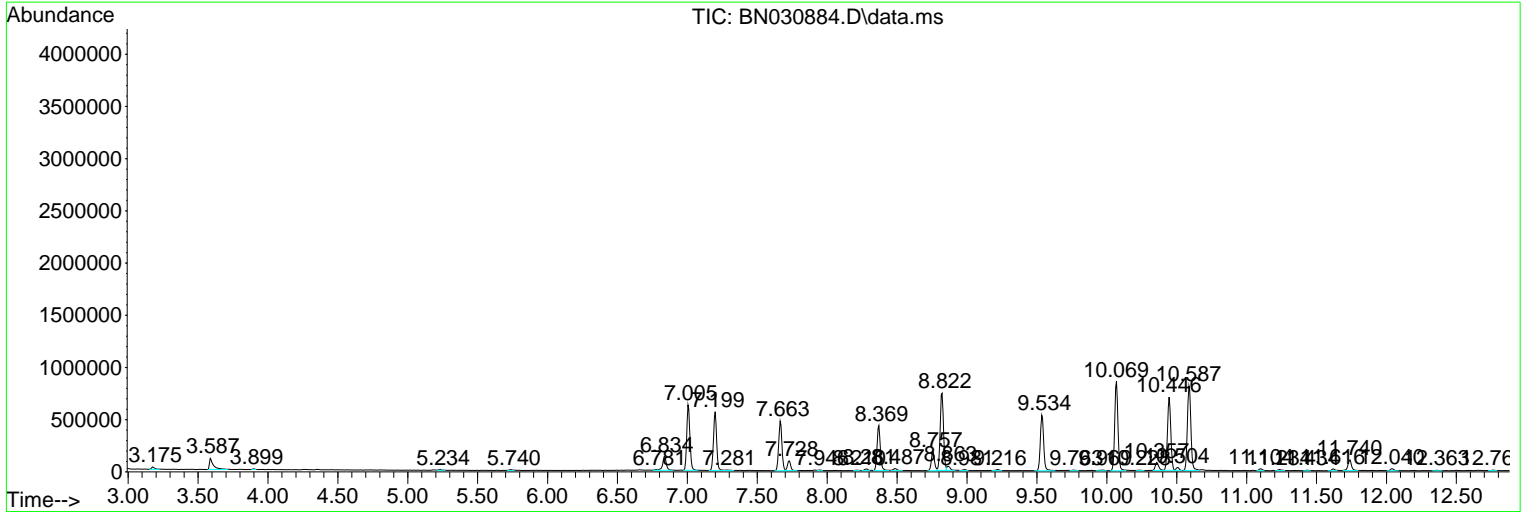
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Instrument :  
 BNA\_N  
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 MCOR79

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_N\Methods\SFAM-EPA-BN032824.MA.M  
 Quant Title : SVOA CALIBRATION

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



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Instrument :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_N\Methods\SFAM-EPA-BN032824.MA.M  
 Quant Title : SVOA CALIBRATION

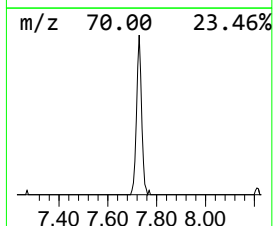
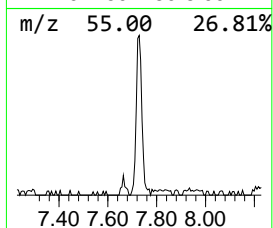
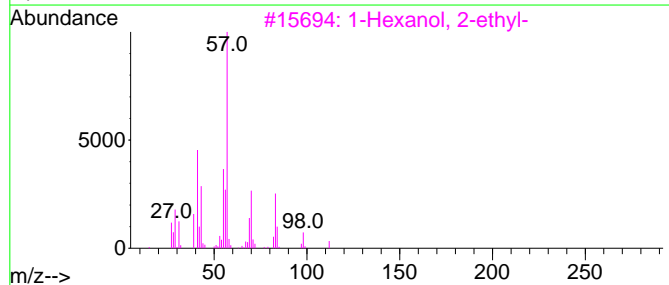
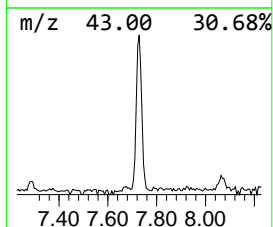
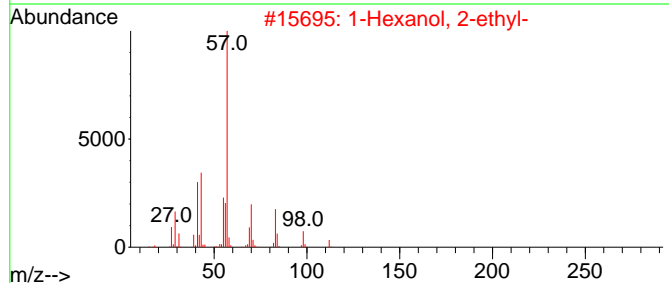
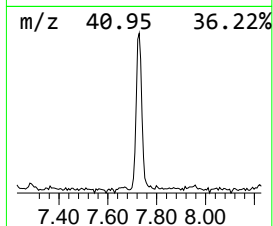
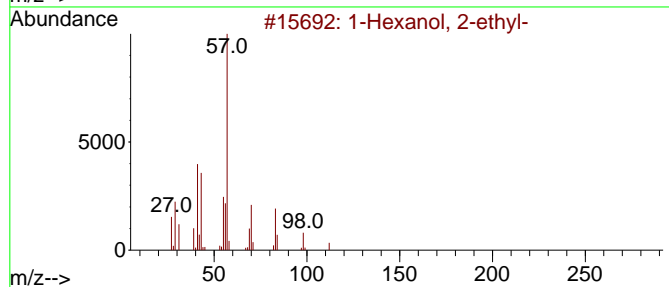
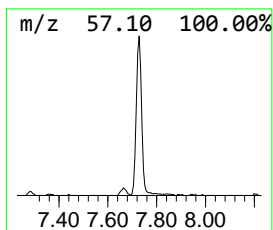
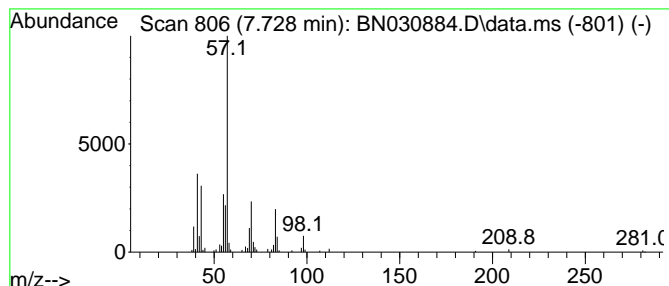
TIC Library : C:\Database\NIST20.L  
 TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.728	3.91 ng/ul	146908	1,4-Dichlorobenzene-d4	7.663

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
3		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
5		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64



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 BNA\_N  
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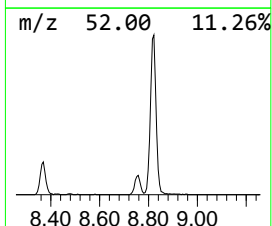
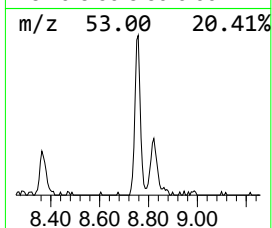
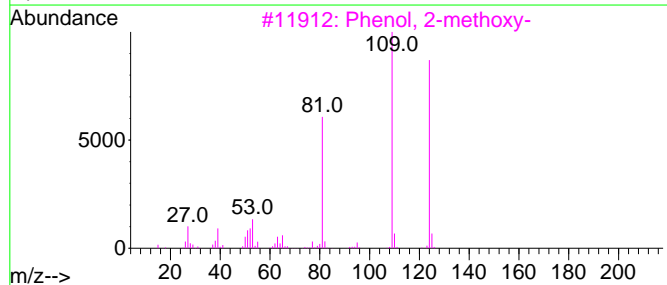
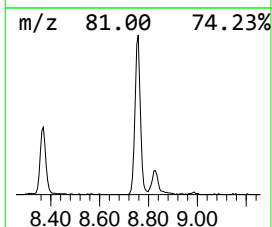
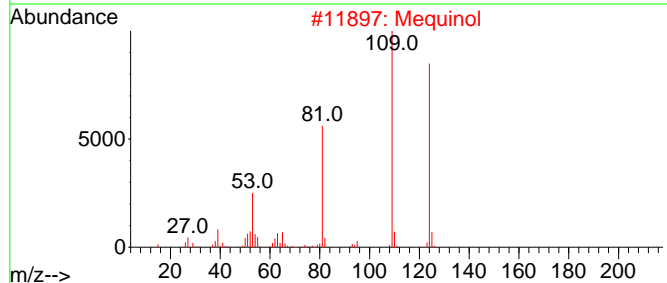
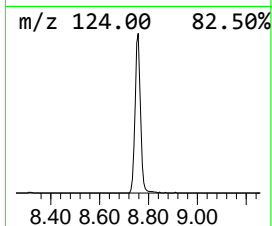
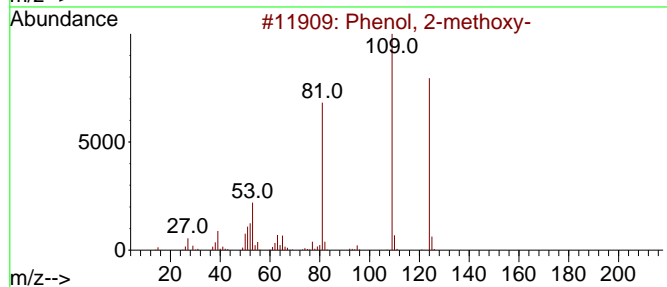
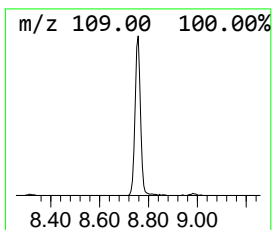
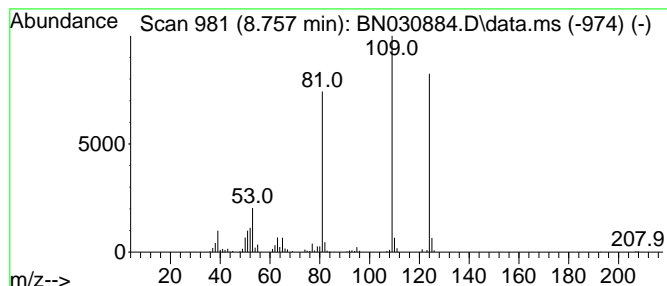
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_N\Methods\SFAM-EPA-BN032824.MA.M  
 Quant Title : SVOA CALIBRATION

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

\*\*\*\*\*  
 Peak Number 2 Phenol, 2-methoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.757	7.94 ng/ul	298525	1,4-Dichlorobenzene-d4	7.663

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	96
2		Mequinol	124	C7H8O2	000150-76-5	91
3		Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	90
4		Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	90
5		Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	89



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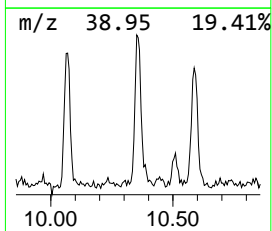
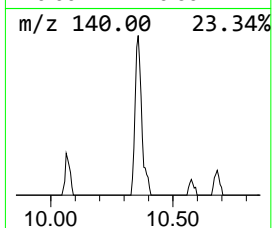
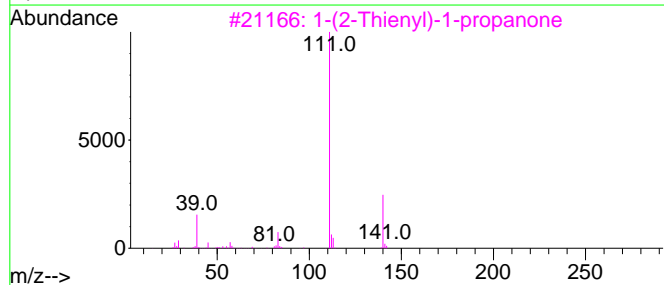
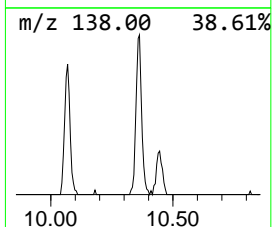
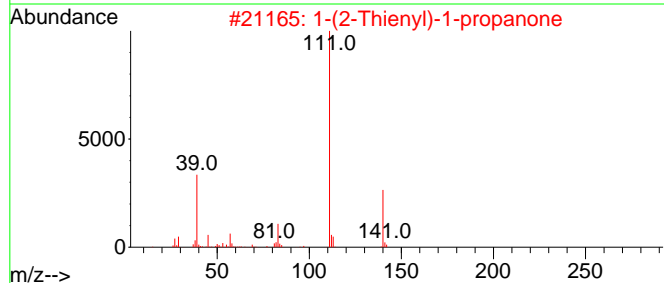
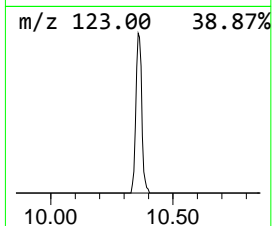
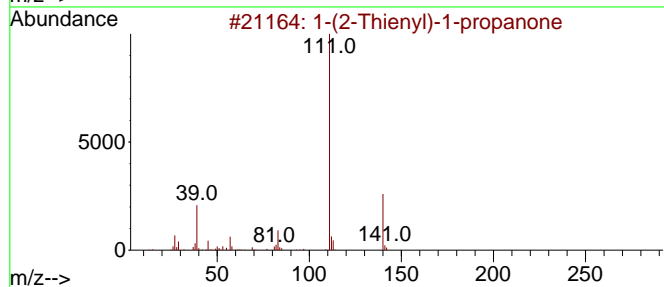
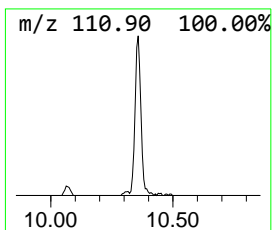
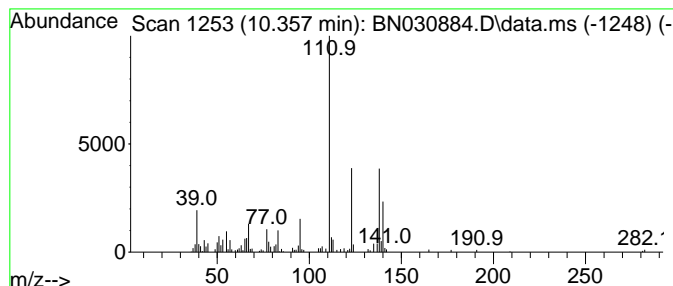
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_N\Methods\SFAM-EPA-BN032824.MA.M  
 Quant Title : SVOA CALIBRATION

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

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 Peak Number 3 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.357	2.31 ng/ul	133231	Naphthalene-d8	10.445

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-(2-Thienyl)-1-propanone	140	C7H8OS	013679-75-9	46
2		1-(2-Thienyl)-1-propanone	140	C7H8OS	013679-75-9	46
3		1-(2-Thienyl)-1-propanone	140	C7H8OS	013679-75-9	38
4		Thiophene, 2-methyl-5-propyl-	140	C8H12S	033933-73-2	38
5		2H-Pyran-2-carboxaldehyde, 3,4-d...	140	C8H12O2	001920-21-4	38



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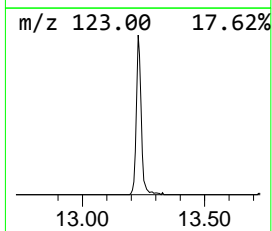
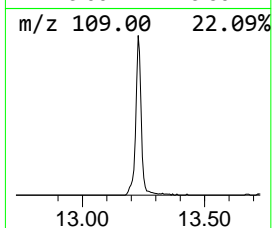
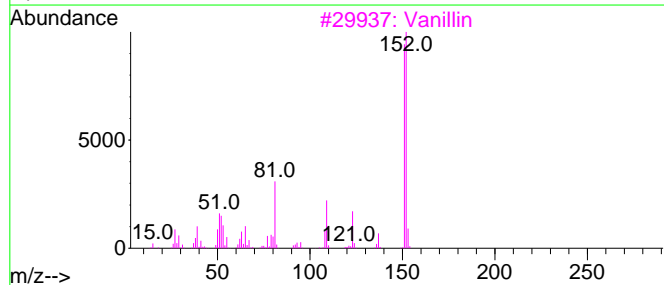
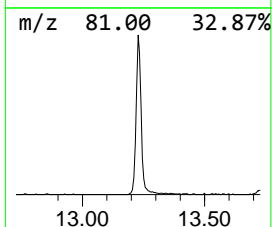
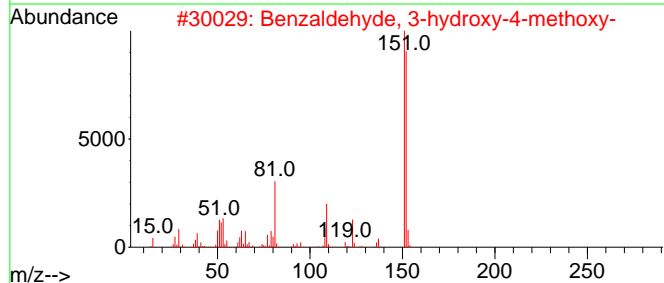
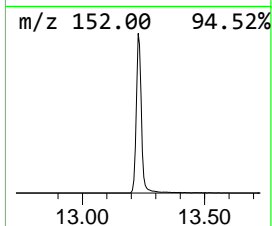
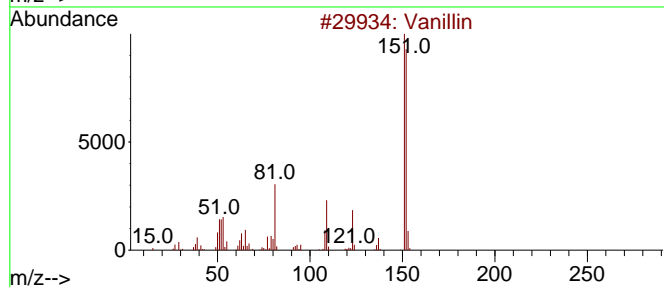
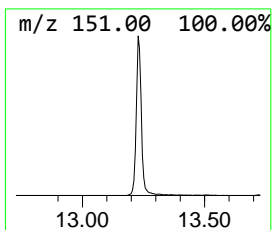
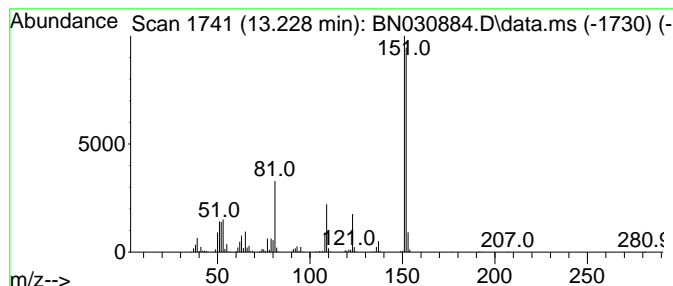
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 TIC Integration Parameters: LSCINT.P

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 Peak Number 4 Vanillin Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.228	9.94 ng/ul	811079	Acenaphthene-d10	14.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Vanillin	152	C8H8O3	000121-33-5	97
2			Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	97
3			Vanillin	152	C8H8O3	000121-33-5	97
4			Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	96
5			Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	96





Data Path : Z:\svoasrv\HPCHEM1\BNA\_N\Data\BN041324\  
 Data File : BN030884.D  
 Acq On : 13 Apr 2024 17:26  
 Operator : MA/JU  
 Sample : P2050-05  
 Misc :  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 BNA\_N  
 ClientSampleId :  
 MCO79

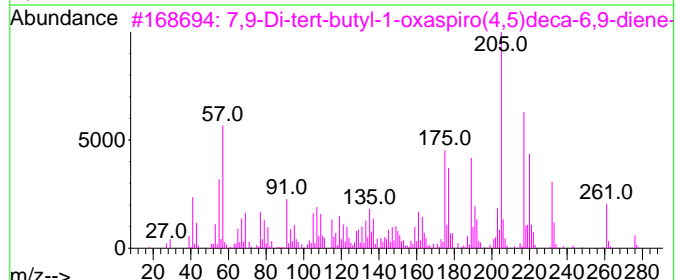
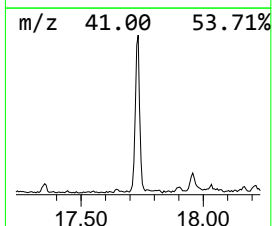
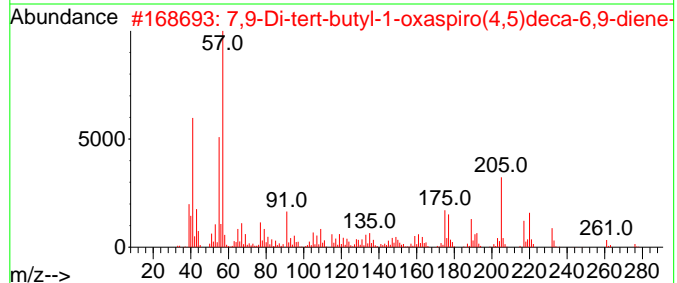
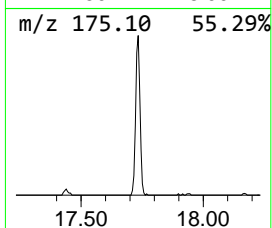
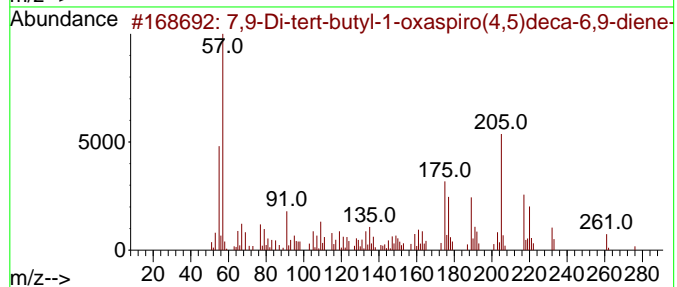
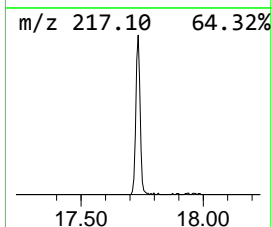
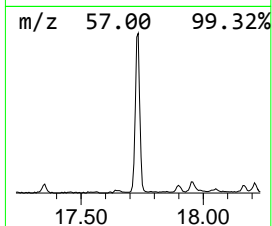
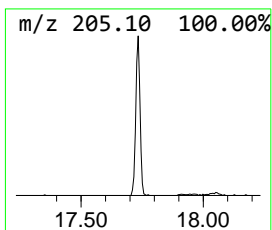
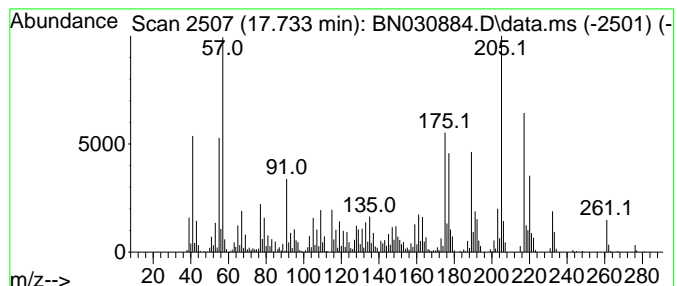
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 Quant Title : SVOA CALIBRATION

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

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 Peak Number 5 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.733	6.64 ng/ul	685463	Phenanthrene-d10	17.057

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	98
3			7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	95
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	45



Data Path : Z:\svoasrv\HPCHEM1\BNA\_N\Data\BN041324\  
Data File : BN030884.D  
Acq On : 13 Apr 2024 17:26  
Operator : MA/JU  
Sample : P2050-05  
Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_N  
ClientSampleId :  
MCOR79

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_N\Methods\SFAM-EPA-BN032824.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
1-Hexanol, 2-et...	7.728	3.9	ng/ul	146908	1	7.663	751725	20.0
Phenol, 2-methoxy-	8.757	7.9	ng/ul	298525	1	7.663	751725	20.0
unknown-01	10.357	2.3	ng/ul	133231	2	10.445	1151260	20.0
Vanillin	13.228	9.9	ng/ul	811079	3	14.310	1632640	20.0
7,9-Di-tert-but...	17.733	6.6	ng/ul	685463	4	17.057	2064840	20.0