

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091324\
 Data File : BG062824.D
 Acq On : 14 Sep 2024 23:16
 Operator : JU/RC
 Sample : P3898-15DL 10X
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DDC88DL

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_G\Methods\SFAM-EPA-BG090924.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG062824.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.781	115	118	122	rVB4	4071	5661	0.41%	0.066%
2	5.021	323	329	336	rBV	29506	49435	3.55%	0.572%
3	6.208	524	531	539	rBV2	7048	13451	0.97%	0.156%
4	7.066	670	677	683	rBV4	11888	25227	1.81%	0.292%
5	7.230	698	705	711	rVB	6683	12517	0.90%	0.145%
6	7.330	718	722	727	rVB2	8855	14121	1.01%	0.163%
7	7.436	736	740	749	rVB6	7965	15184	1.09%	0.176%
8	7.530	752	756	765	rVV5	11472	23777	1.71%	0.275%
9	7.900	812	819	826	rBV	154722	272684	19.56%	3.156%
10	7.965	828	830	835	rVB4	3770	5291	0.38%	0.061%
11	8.323	886	891	896	rBV2	14658	25125	1.80%	0.291%
12	8.376	896	900	905	rVV	13526	20218	1.45%	0.234%
13	8.435	906	910	917	rVB4	5160	10451	0.75%	0.121%
14	8.499	917	921	925	rVB3	5274	7227	0.52%	0.084%
15	8.540	925	928	930	rBV3	4565	6949	0.50%	0.080%
16	8.599	935	938	944	rVB5	10123	18236	1.31%	0.211%
17	8.670	945	950	954	rBV2	6108	11777	0.84%	0.136%
18	8.893	983	988	996	rVB3	20800	36559	2.62%	0.423%
19	9.010	999	1008	1013	rBV3	14436	26633	1.91%	0.308%
20	9.052	1013	1015	1021	rVV3	7671	11577	0.83%	0.134%
21	9.134	1023	1029	1033	rVB	20423	30644	2.20%	0.355%
22	9.480	1084	1088	1092	rVB4	8416	13304	0.95%	0.154%
23	9.680	1116	1122	1128	rBV4	4168	7524	0.54%	0.087%
24	9.774	1131	1138	1144	rVV7	6854	15186	1.09%	0.176%
25	9.921	1159	1163	1168	rVB5	6987	10444	0.75%	0.121%
26	9.986	1170	1174	1179	rVB4	4083	7326	0.53%	0.085%
27	10.186	1201	1208	1213	rBV4	14685	26431	1.90%	0.306%
28	10.321	1227	1231	1236	rVB2	10916	15256	1.09%	0.177%
29	10.567	1269	1273	1276	rBV4	3405	5919	0.42%	0.069%
30	10.685	1284	1293	1302	rBV2	488310	890997	63.93%	10.314%
31	10.808	1306	1314	1324	rVV2	84347	161111	11.56%	1.865%
32	10.891	1325	1328	1334	rVV3	7804	12789	0.92%	0.148%
33	10.979	1334	1343	1348	rVV7	15269	33904	2.43%	0.392%
34	11.084	1356	1361	1368	rVB4	9172	15455	1.11%	0.179%
35	11.196	1371	1380	1389	rBV	53024	91882	6.59%	1.064%
36	11.584	1440	1446	1449	rBV2	26320	45943	3.30%	0.532%

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Integration Parameters: LSCINT.P

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37	11.719	1464	1469	1476	rVB2	13173	20330	1.46%	0.235%
38	11.813	1479	1485	1489	rVV4	8303	13631	0.98%	0.158%
39	11.931	1499	1505	1515	rVB6	18573	41428	2.97%	0.480%
40	12.025	1515	1521	1530	rBV4	8758	17086	1.23%	0.198%
41	12.107	1530	1535	1540	rBV4	25835	42229	3.03%	0.489%
42	12.195	1545	1550	1554	rVV4	10317	17614	1.26%	0.204%
43	12.230	1554	1556	1560	rVB3	4840	5749	0.41%	0.067%
44	12.348	1571	1576	1582	rVB2	5185	9388	0.67%	0.109%
45	12.448	1588	1593	1596	rBV6	6172	11579	0.83%	0.134%
46	12.518	1600	1605	1612	rBV3	78117	122244	8.77%	1.415%
47	12.771	1646	1648	1654	rVB4	3609	6128	0.44%	0.071%
48	12.871	1660	1665	1670	rBV4	7970	11880	0.85%	0.138%
49	12.959	1677	1680	1687	rVB4	8538	14361	1.03%	0.166%
50	13.053	1690	1696	1699	rBV4	4480	9036	0.65%	0.105%
51	13.100	1699	1704	1710	rVB	26348	36609	2.63%	0.424%
52	13.159	1710	1714	1719	rBV5	3794	6790	0.49%	0.079%
53	13.358	1743	1748	1754	rBV3	13525	21795	1.56%	0.252%
54	13.417	1754	1758	1760	rBV4	3796	5184	0.37%	0.060%
55	13.576	1780	1785	1791	rVB4	21545	37150	2.67%	0.430%
56	13.705	1798	1807	1811	rBV5	17143	35839	2.57%	0.415%
57	13.852	1827	1832	1833	rBV4	5949	7437	0.53%	0.086%
58	13.934	1842	1846	1851	rVB	25159	36526	2.62%	0.423%
59	14.222	1889	1895	1898	rBV2	27113	42259	3.03%	0.489%
60	14.257	1898	1901	1907	rVB	19462	25812	1.85%	0.299%
61	14.334	1910	1914	1916	rVB3	4152	5438	0.39%	0.063%
62	14.428	1924	1930	1935	rBV3	14569	24010	1.72%	0.278%
63	14.475	1935	1938	1941	rVV4	6975	8167	0.59%	0.095%
64	14.527	1941	1947	1954	rVV	427959	659090	47.29%	7.629%
65	14.739	1978	1983	1986	rBV5	9155	15768	1.13%	0.183%
66	14.927	2012	2015	2020	rVB6	5838	8090	0.58%	0.094%
67	15.003	2023	2028	2030	rBV3	5140	7599	0.55%	0.088%
68	15.050	2032	2036	2044	rVV6	7945	16124	1.16%	0.187%
69	15.156	2048	2054	2060	rVV	46958	78512	5.63%	0.909%
70	15.256	2064	2071	2076	rBV7	15185	25903	1.86%	0.300%
71	15.385	2089	2093	2098	rVB2	15848	20963	1.50%	0.243%
72	15.520	2111	2116	2123	rVB	42620	63354	4.55%	0.733%
73	15.626	2125	2134	2138	rBV9	11749	29211	2.10%	0.338%
74	15.791	2153	2162	2165	rBV6	13473	26167	1.88%	0.303%
75	15.885	2174	2178	2185	rBV2	22342	32743	2.35%	0.379%
76	16.243	2235	2239	2242	rBV	17486	24828	1.78%	0.287%

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77	16.343	2251	2256	2259	rBV6	8045	12732	0.91%	0.147%
78	16.449	2271	2274	2278	rBV4	3907	5027	0.36%	0.058%
79	16.496	2280	2282	2287	rVB6	7254	8729	0.63%	0.101%
80	16.925	2349	2355	2368	rBV	552388	850986	61.06%	9.851%
81	17.036	2371	2374	2378	rVV3	21389	31366	2.25%	0.363%
82	17.089	2380	2383	2388	rVV5	13411	23363	1.68%	0.270%
83	17.160	2392	2395	2399	rVB4	8070	9881	0.71%	0.114%
84	17.271	2408	2414	2422	rBV	636129	988023	70.89%	11.437%
85	17.371	2426	2431	2437	rVV3	54860	80042	5.74%	0.927%
86	17.418	2437	2439	2443	rBV4	3950	4811	0.35%	0.056%
87	17.459	2443	2446	2449	rBV3	11707	13268	0.95%	0.154%
88	17.571	2462	2465	2470	rVB6	9332	14656	1.05%	0.170%
89	17.777	2496	2500	2503	rBV2	16772	19583	1.41%	0.227%
90	18.164	2563	2566	2570	rBV5	9339	11610	0.83%	0.134%
91	18.464	2614	2617	2621	rVB3	13831	16251	1.17%	0.188%
92	18.828	2674	2679	2682	rBV6	3316	5795	0.42%	0.067%
93	18.869	2683	2686	2689	rVV4	4020	5575	0.40%	0.065%
94	19.099	2722	2725	2728	rVB2	12169	12743	0.91%	0.148%
95	19.663	2817	2821	2828	rVB	81032	116663	8.37%	1.350%
96	20.209	2911	2914	2918	rVB3	9832	11150	0.80%	0.129%
97	20.703	2995	2998	3001	rBV4	8871	9184	0.66%	0.106%
98	21.190	3078	3081	3091	rVB5	22761	42149	3.02%	0.488%
99	21.519	3131	3137	3149	rVB2	810156	1311212	94.08%	15.178%
100	24.580	3648	3658	3670	rBV	501277	1393782	100.00%	16.134%

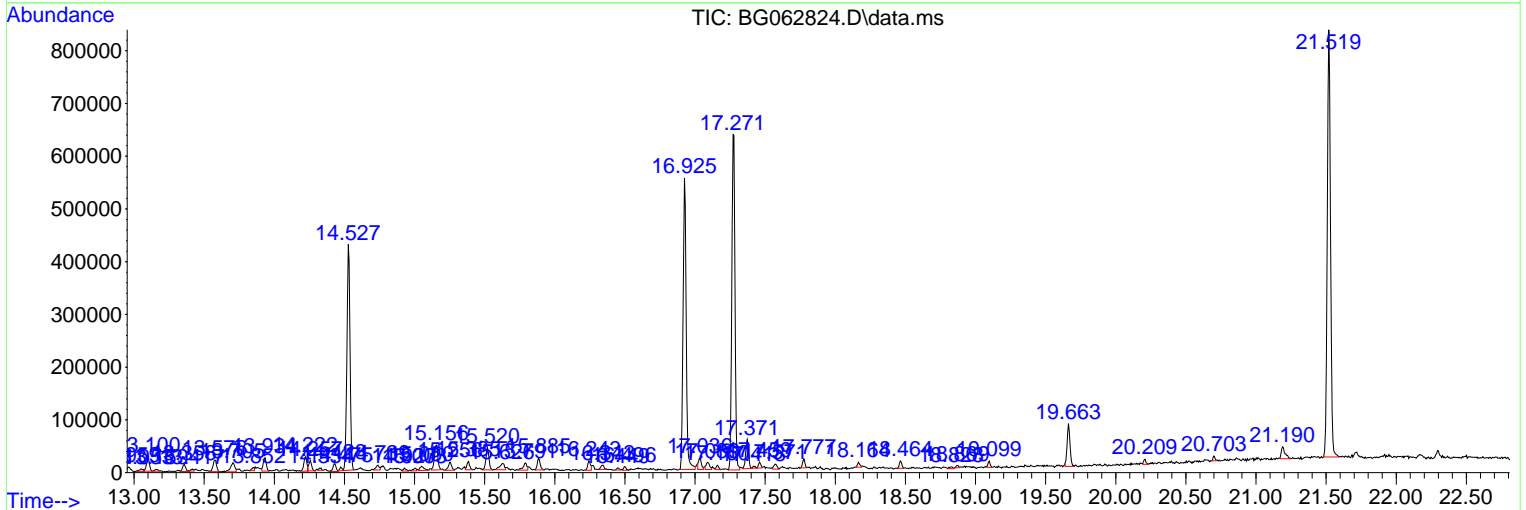
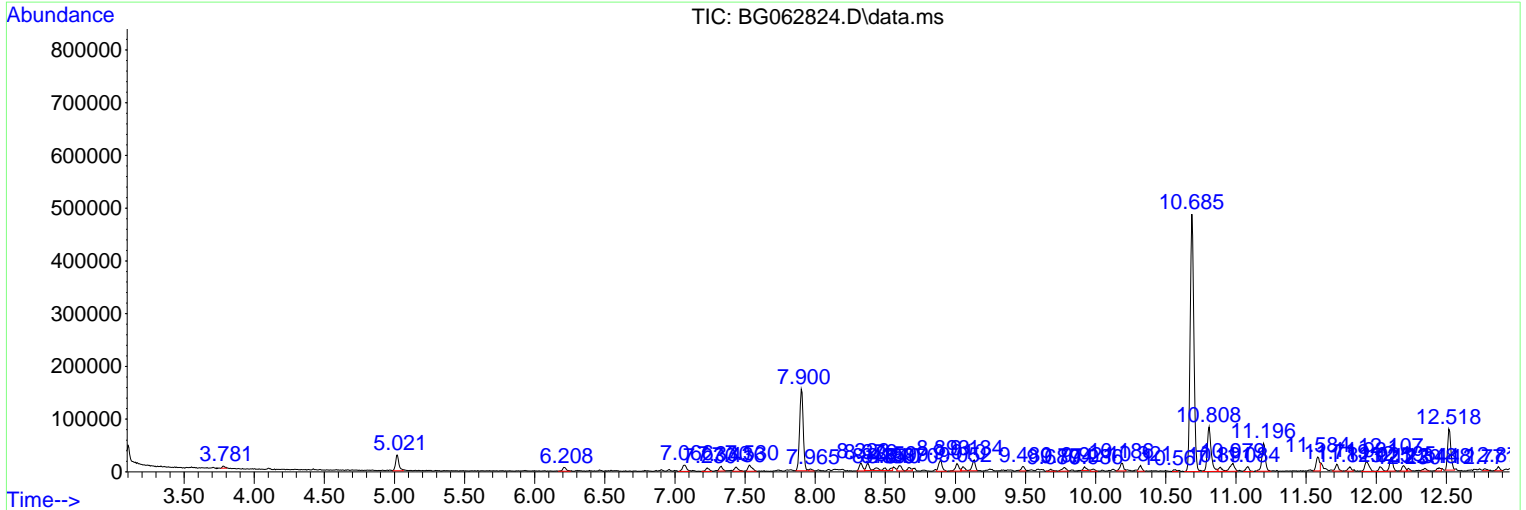
Sum of corrected areas: 8638847

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG090924.MA.M
 Quant Title : SVOA CALIBRATION

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



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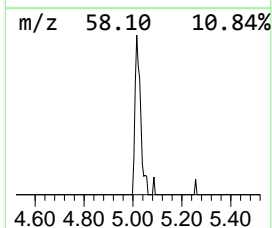
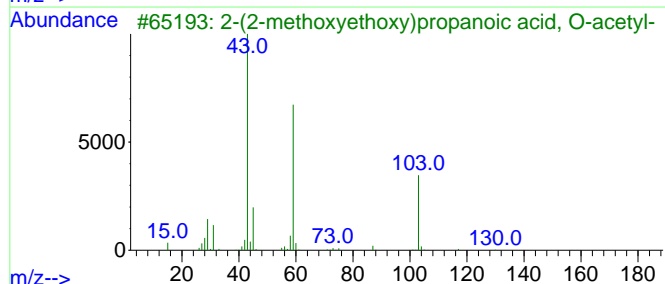
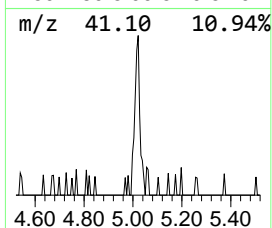
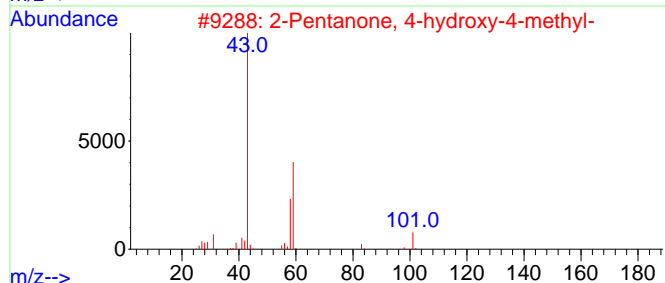
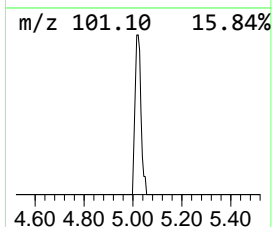
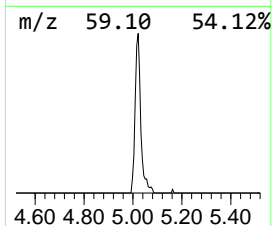
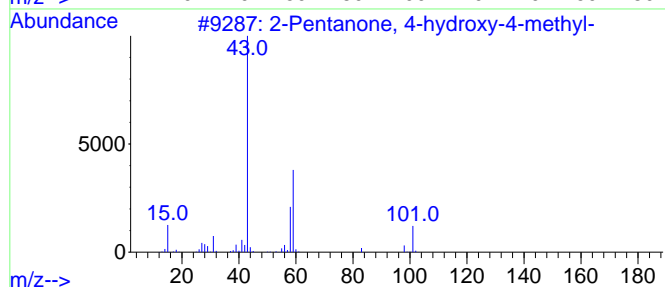
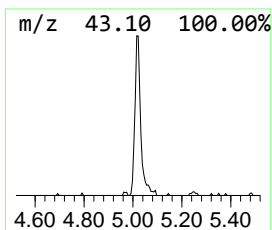
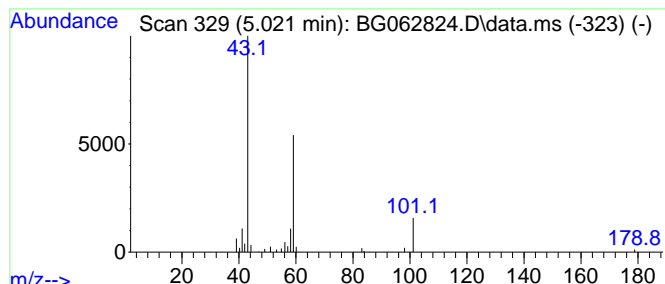
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG090924.MA.M
 Quant Title : SVOA CALIBRATION

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

 Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.021	3.63 ng/ul	49435	1,4-Dichlorobenzene-d4	7.900

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
3			2-(2-methoxyethoxy)propanoic aci...	190	C8H14O5	1000506-61-7	45
4			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
5			3-Hexanol	102	C6H14O	000623-37-0	33



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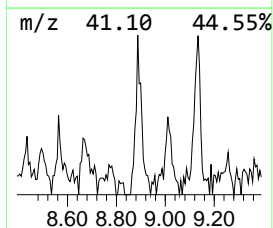
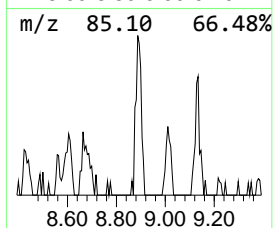
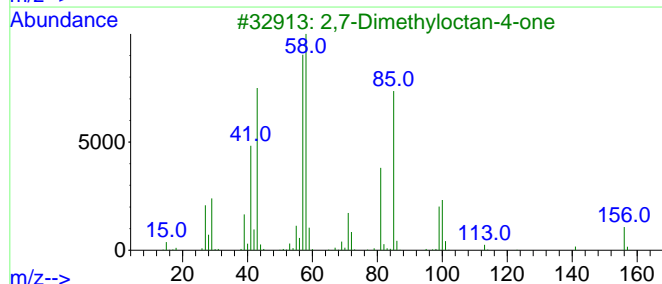
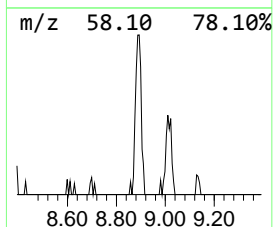
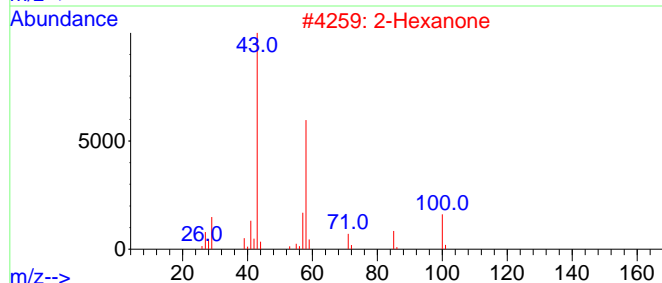
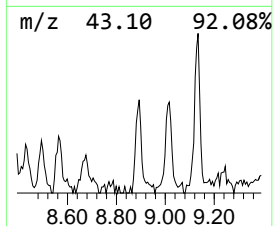
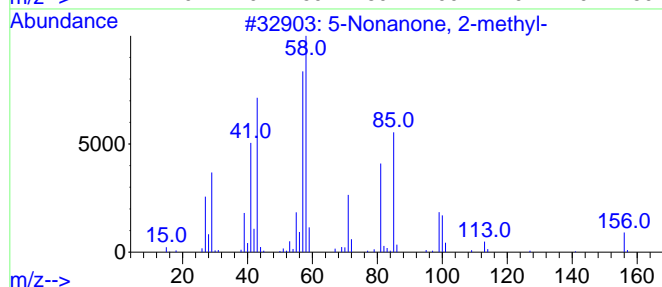
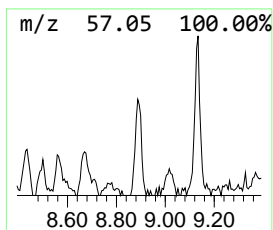
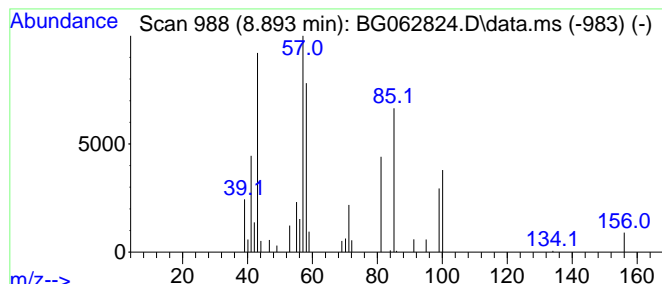
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG090924.MA.M
 Quant Title : SVOA CALIBRATION

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

 Peak Number 2 5-Nonanone, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.893	2.68 ng/ul	36559	1,4-Dichlorobenzene-d4	7.900

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Nonanone, 2-methyl-	156	C10H20O	022287-02-1	64
2		2-Hexanone	100	C6H12O	000591-78-6	43
3		2,7-Dimethyloctan-4-one	156	C10H20O	059387-92-7	38
4		4-Octanone	128	C8H16O	000589-63-9	38
5		S-[2-[N,N-Dimethylamino]ethyl]mo...	261	C10H19N3O3S	1000212-14-3	35



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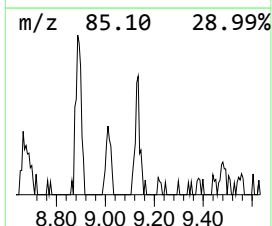
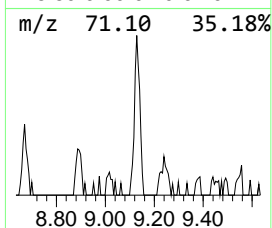
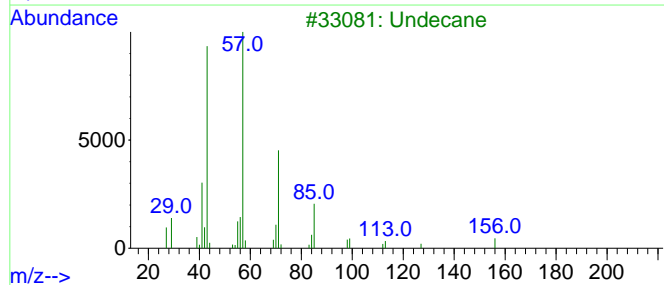
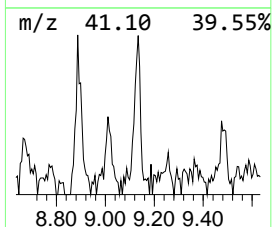
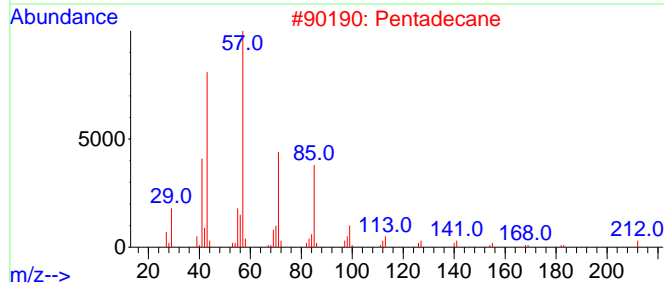
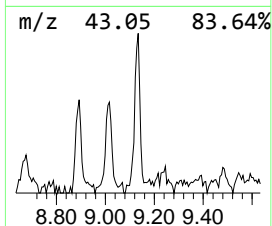
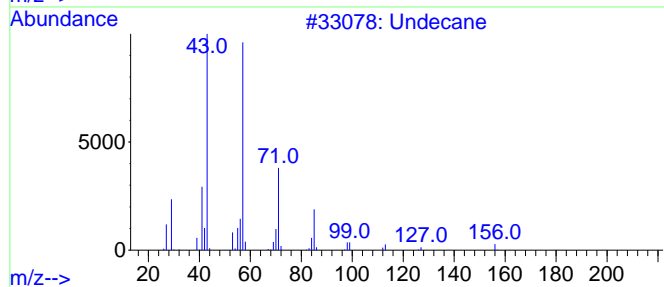
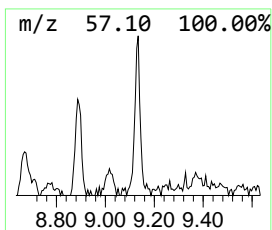
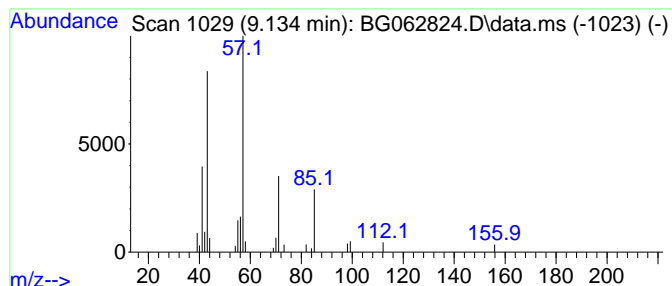
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG090924.MA.M
 Quant Title : SVOA CALIBRATION

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

 Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.134	2.25 ng/ul	30644	1,4-Dichlorobenzene-d4	7.900

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	80
2			Pentadecane	212	C15H32	000629-62-9	78
3			Undecane	156	C11H24	001120-21-4	64
4			Decane	142	C10H22	000124-18-5	56
5			Decane	142	C10H22	000124-18-5	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091324\
 Data File : BG062824.D
 Acq On : 14 Sep 2024 23:16
 Operator : JU/RC
 Sample : P3898-15DL 10X
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DDC88DL

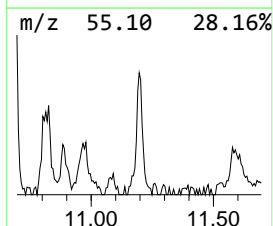
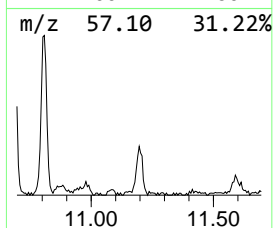
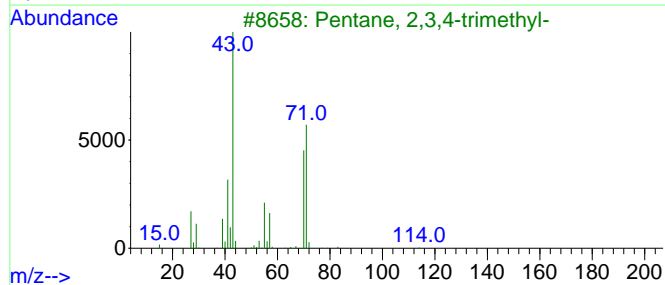
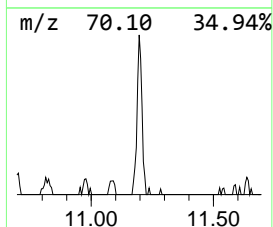
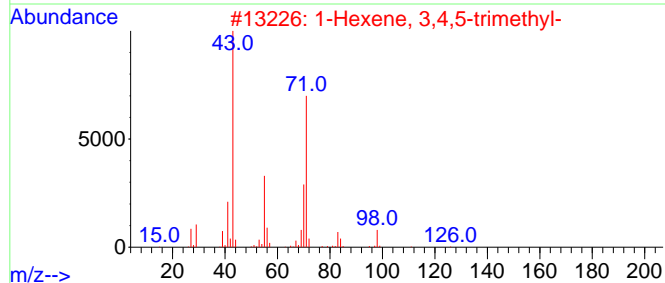
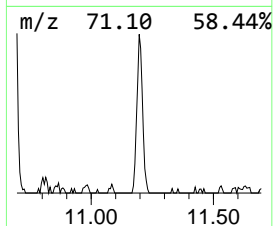
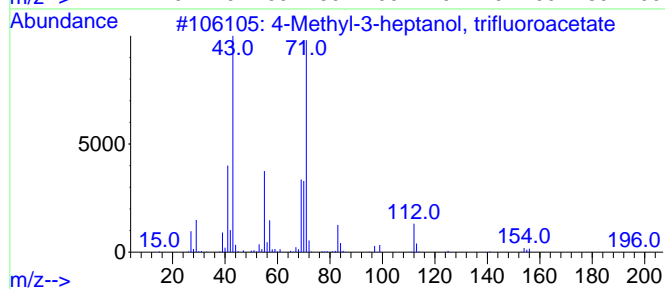
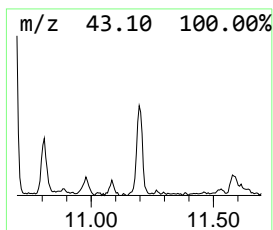
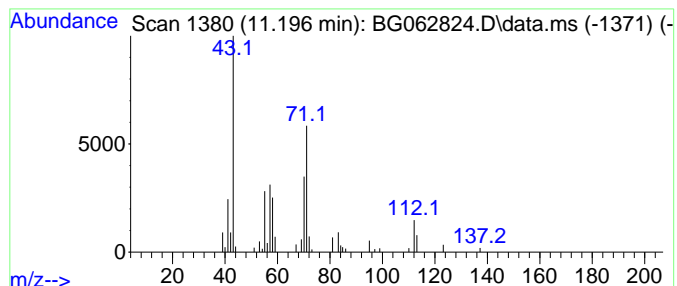
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 Quant Title : SVOA CALIBRATION

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

 Peak Number 4 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.196	2.06 ng/ul	91882	Naphthalene-d8	10.691

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Methyl-3-heptanol, trifluoroac...	226	C10H17F3O2	1000365-51-8	47
2		1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	43
3		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	38
4		4-Methyl-3-heptanol, pentafluoro...	276	C11H17F5O2	1000365-51-7	38
5		Heptane, 3,3-dimethyl-	128	C9H20	004032-86-4	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091324\
 Data File : BG062824.D
 Acq On : 14 Sep 2024 23:16
 Operator : JU/RC
 Sample : P3898-15DL 10X
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DDC88DL

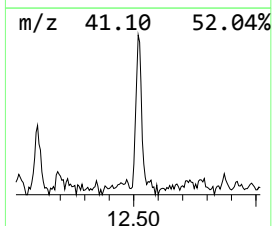
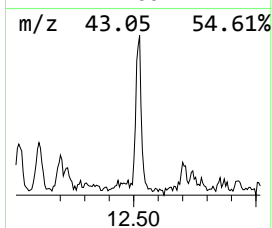
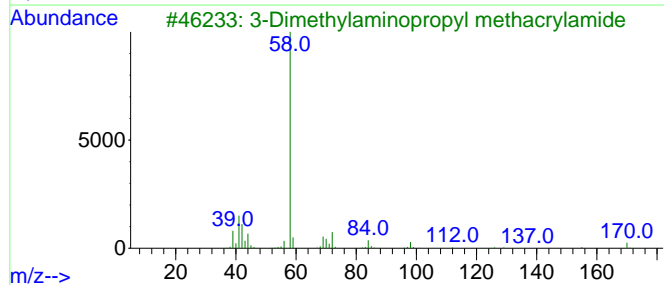
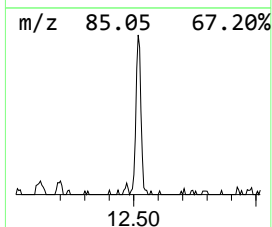
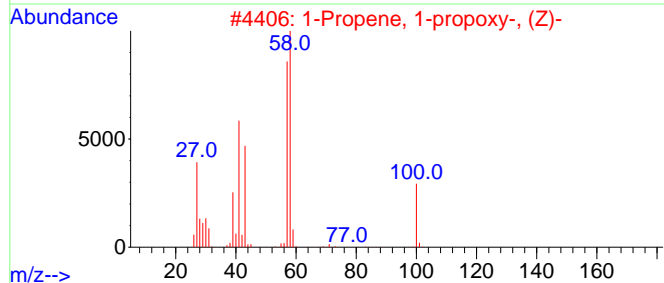
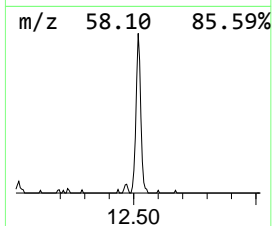
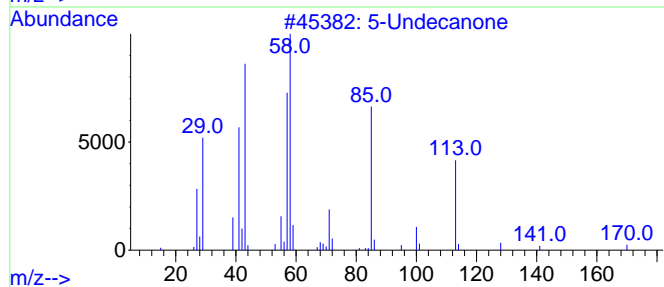
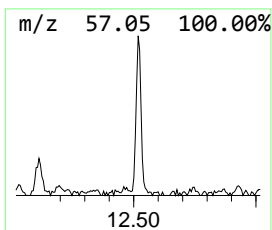
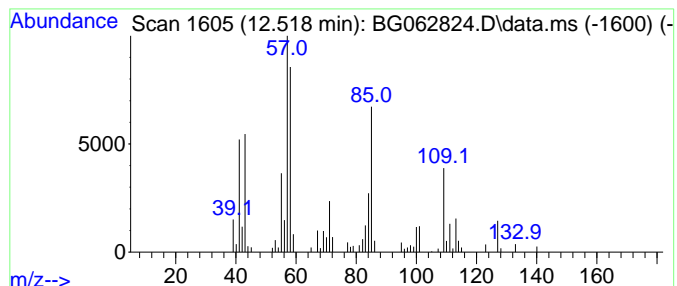
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 Quant Title : SVOA CALIBRATION

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

 Peak Number 5 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.518	2.74 ng/ul	122244	Naphthalene-d8	10.691

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Undecanone	170	C11H22O	033083-83-9	47
2			1-Propene, 1-propoxy-, (Z)-	100	C6H12O	014360-78-2	25
3			3-Dimethylaminopropyl methacryla...	170	C9H18N2O	005205-93-6	22
4			S-[2-[N,N-Dimethylamino]ethyl]mo...	261	C10H19N3O3S	1000212-14-3	22
5			Cyclohexane, 1,3-dimethoxy-5-met...	158	C9H18O2	030363-82-7	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091324\
 Data File : BG062824.D
 Acq On : 14 Sep 2024 23:16
 Operator : JU/RC
 Sample : P3898-15DL 10X
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DDC88DL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG090924.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-Pentanone, 4-...	5.021	3.6	ng/u1	49435	1	7.900	272684	20.0
5-Nonanone, 2-m...	8.893	2.7	ng/u1	36559	1	7.900	272684	20.0
(DEL) Alkane: S...	9.134	2.3	ng/u1	30644	1	7.900	272684	20.0
unknown-01	11.196	2.1	ng/u1	91882	2	10.691	890997	20.0
unknown-02	12.518	2.7	ng/u1	122244	2	10.691	890997	20.0