

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN041423\
 Data File : BN024895.D
 Acq On : 14 Apr 2023 13:25
 Operator : CG/JU
 Sample : 02252-17
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 COMF3

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: BN024895.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.305	17	20	29	rVB	60052	93381	0.92%	0.100%
2	3.746	94	95	115	rBV	140820	262970	2.60%	0.281%
3	3.975	128	134	139	rVB7	11222	19922	0.20%	0.021%
4	4.070	146	150	160	rVB2	23745	42462	0.42%	0.045%
5	4.446	210	214	221	rVB6	12134	22724	0.22%	0.024%
6	5.452	381	385	392	rVB	19351	30177	0.30%	0.032%
7	5.969	470	473	479	rBV6	13883	21813	0.22%	0.023%
8	6.916	630	634	643	rBV4	21334	42299	0.42%	0.045%
9	7.034	649	654	657	rBV3	15576	25462	0.25%	0.027%
10	7.099	657	665	675	rVB	296840	503595	4.98%	0.537%
11	7.263	687	693	707	rVB	1124794	1798820	17.79%	1.920%
12	7.463	720	727	736	rBV	1048996	1702149	16.83%	1.817%
13	7.940	801	808	814	rBV	1106383	1748724	17.29%	1.866%
14	7.999	814	818	826	rVB	147365	221745	2.19%	0.237%
15	8.505	897	904	908	rBV6	12836	28470	0.28%	0.030%
16	8.557	908	913	918	rVB	27093	41948	0.41%	0.045%
17	8.652	923	929	939	rVV	858988	1359863	13.45%	1.451%
18	8.769	944	949	956	rVB	38339	60937	0.60%	0.065%
19	9.046	988	996	1001	rBV	297825	487573	4.82%	0.520%
20	9.110	1001	1007	1012	rVV	1431312	2374734	23.48%	2.535%
21	9.157	1012	1015	1020	rVV	67804	105663	1.04%	0.113%
22	9.216	1020	1025	1030	rVV2	31036	62579	0.62%	0.067%
23	9.269	1030	1034	1042	rVB3	36680	59998	0.59%	0.064%
24	9.834	1121	1130	1142	rBV	1178288	1944589	19.23%	2.075%
25	9.981	1148	1155	1160	rBV4	11603	25479	0.25%	0.027%
26	10.057	1163	1168	1173	rVV3	27681	44312	0.44%	0.047%
27	10.269	1199	1204	1208	rBV6	10736	19355	0.19%	0.021%
28	10.369	1214	1221	1231	rBV	1605827	2651575	26.22%	2.830%
29	10.528	1242	1248	1253	rBV8	10463	20075	0.20%	0.021%
30	10.657	1258	1270	1279	rVV2	146498	294025	2.91%	0.314%
31	10.752	1279	1286	1292	rVV	1555169	2620377	25.91%	2.797%
32	10.810	1292	1296	1301	rVV	61745	97331	0.96%	0.104%
33	10.893	1302	1310	1321	rVV	1053781	1798525	17.78%	1.920%
34	10.981	1322	1325	1333	rVB4	11463	20816	0.21%	0.022%
35	11.410	1393	1398	1406	rVB2	24337	49151	0.49%	0.052%
36	11.540	1415	1420	1428	rBV	89589	163668	1.62%	0.175%

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

37	11.734	1449	1453	1457	rVV4	13374	19984	0.20%	0.021%
38	11.922	1480	1485	1489	rBV	36314	58253	0.58%	0.062%
39	12.040	1495	1505	1516	rBV	317364	529595	5.24%	0.565%
40	12.340	1551	1556	1562	rVV2	37260	66104	0.65%	0.071%
41	12.793	1627	1633	1639	rBV10	10736	22672	0.22%	0.024%
42	13.093	1679	1684	1692	rVB5	13067	21494	0.21%	0.023%
43	13.193	1696	1701	1712	rVB8	12865	32478	0.32%	0.035%
44	13.504	1746	1754	1760	rBV	1219997	1777092	17.57%	1.897%
45	13.551	1760	1762	1769	rVV5	37054	53492	0.53%	0.057%
46	13.622	1769	1774	1783	rVB	62372	98428	0.97%	0.105%
47	13.993	1831	1837	1850	rVV	3215612	4373702	43.24%	4.668%
48	14.281	1879	1886	1892	rBV	3440931	4960880	49.05%	5.295%
49	14.369	1897	1901	1907	rVV3	16792	27527	0.27%	0.029%
50	14.445	1909	1914	1925	rVB2	36906	68608	0.68%	0.073%
51	14.587	1927	1938	1944	rBV	2412558	3548270	35.08%	3.787%
52	14.628	1944	1945	1947	rVV2	29798	23834	0.24%	0.025%
53	14.663	1947	1951	1958	rVB	54565	82302	0.81%	0.088%
54	14.781	1965	1971	1979	rBV	266127	436835	4.32%	0.466%
55	14.840	1979	1981	1988	rVB3	18404	27459	0.27%	0.029%
56	14.987	2003	2006	2012	rBV6	16433	25789	0.25%	0.028%
57	15.257	2046	2052	2059	rBV	100201	148075	1.46%	0.158%
58	15.392	2069	2075	2081	rVV5	13815	32809	0.32%	0.035%
59	15.575	2099	2106	2113	rBV	4321816	6405128	63.33%	6.836%
60	15.634	2113	2116	2120	rVB5	15525	18877	0.19%	0.020%
61	15.692	2120	2126	2139	rBV	1740820	2312970	22.87%	2.469%
62	15.804	2139	2145	2152	rBV6	41532	95237	0.94%	0.102%
63	15.939	2163	2168	2171	rBV	55298	82397	0.81%	0.088%
64	16.145	2200	2203	2209	rVB7	19128	28966	0.29%	0.031%
65	16.216	2209	2215	2221	rBV	49595	76141	0.75%	0.081%
66	17.034	2346	2354	2359	rBV2	54511	89366	0.88%	0.095%
67	17.334	2398	2405	2412	rVB	2937305	4183442	41.36%	4.465%
68	17.434	2415	2422	2435	rVV	5185761	7479864	73.95%	7.983%
69	17.575	2442	2446	2449	rBV3	14089	19182	0.19%	0.020%
70	17.610	2449	2452	2457	rVB	15918	21510	0.21%	0.023%
71	17.710	2465	2469	2472	rBV2	15047	19093	0.19%	0.020%
72	17.798	2479	2484	2493	rBV3	49268	114432	1.13%	0.122%
73	17.916	2500	2504	2507	rBV5	15717	22800	0.23%	0.024%
74	17.957	2507	2511	2513	rVV	29690	37550	0.37%	0.040%
75	17.998	2513	2518	2527	rVB	1143811	1450362	14.34%	1.548%
76	18.104	2532	2536	2542	rBV2	32097	53893	0.53%	0.058%

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 Title : SVOA CALIBRATION

77	18.169	2544	2547	2550	rBV3	21806	25050	0.25%	0.027%
78	18.222	2551	2556	2565	rBV	220340	348615	3.45%	0.372%
79	18.304	2565	2570	2579	rBV2	97243	191762	1.90%	0.205%
80	18.433	2589	2592	2596	rBV5	23874	31761	0.31%	0.034%
81	18.480	2597	2600	2608	rVB5	27873	45834	0.45%	0.049%
82	18.963	2679	2682	2697	rVB	136405	272689	2.70%	0.291%
83	19.080	2698	2702	2708	rBV2	74856	116355	1.15%	0.124%
84	19.286	2734	2737	2744	rVB2	67356	91817	0.91%	0.098%
85	19.357	2745	2749	2754	rBV	69823	118758	1.17%	0.127%
86	19.498	2769	2773	2781	rBV	211204	298565	2.95%	0.319%
87	19.575	2782	2786	2795	rVB	103911	191047	1.89%	0.204%
88	19.727	2804	2812	2819	rBV	6916089	9038460	89.36%	9.647%
89	19.822	2825	2828	2837	rVB	59073	84285	0.83%	0.090%
90	19.969	2848	2853	2859	rBV	110118	206364	2.04%	0.220%
91	20.498	2939	2943	2949	rBV	144086	202677	2.00%	0.216%
92	20.733	2980	2983	2987	rBV	132053	151483	1.50%	0.162%
93	20.992	3024	3027	3038	rVB	203121	363718	3.60%	0.388%
94	21.322	3080	3083	3087	rBV	130565	179904	1.78%	0.192%
95	21.527	3113	3118	3137	rVB	3948732	5385199	53.24%	5.748%
96	21.780	3158	3161	3167	rBV2	116847	153865	1.52%	0.164%
97	23.816	3499	3507	3521	rVB2	4752685	10114123	100.00%	10.795%
98	23.968	3526	3533	3544	rVB2	2213183	4789575	47.36%	5.112%
99	24.574	3632	3636	3645	rVB	344583	719137	7.11%	0.768%
100	25.433	3777	3782	3790	rVB2	325050	759774	7.51%	0.811%

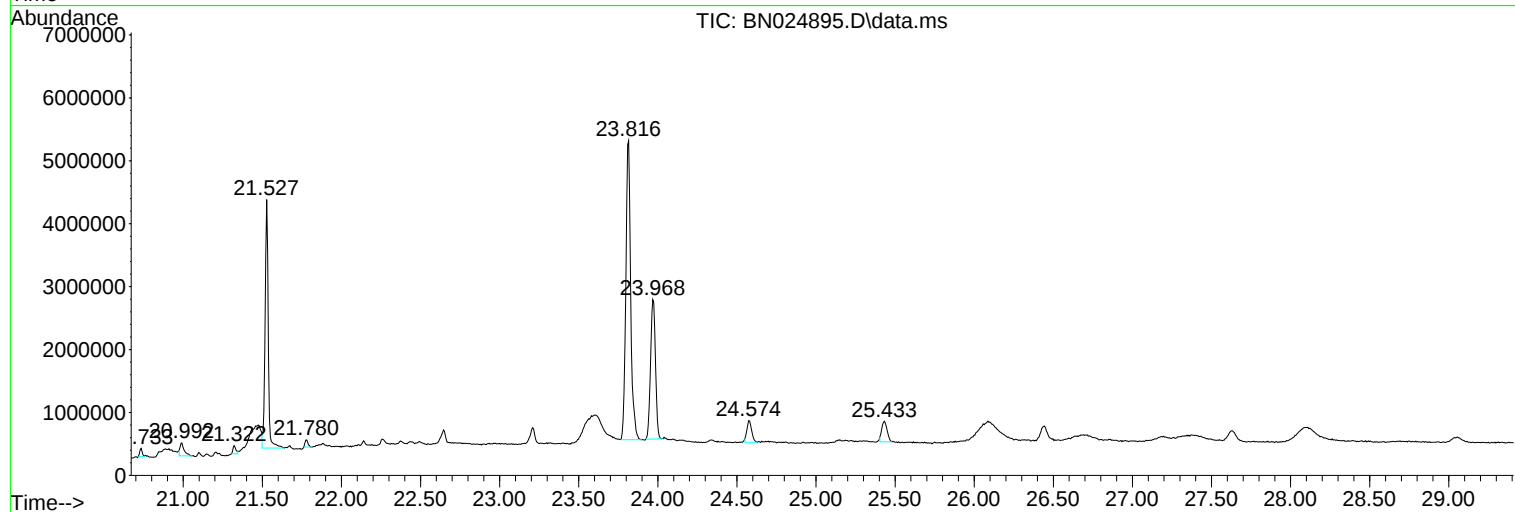
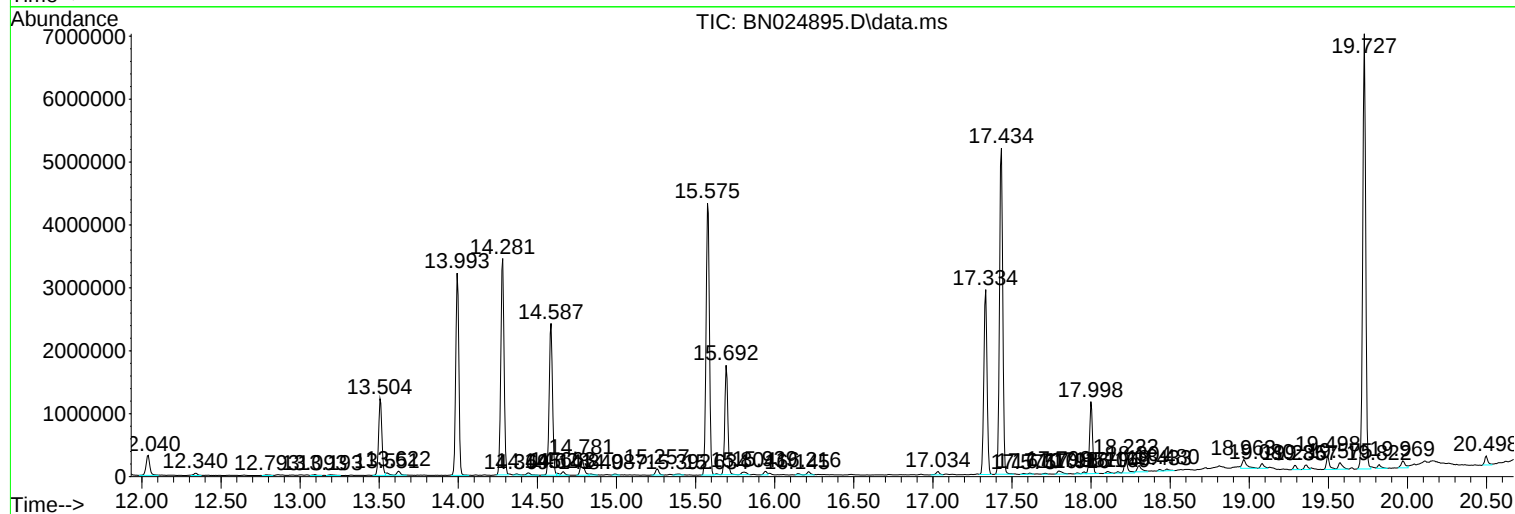
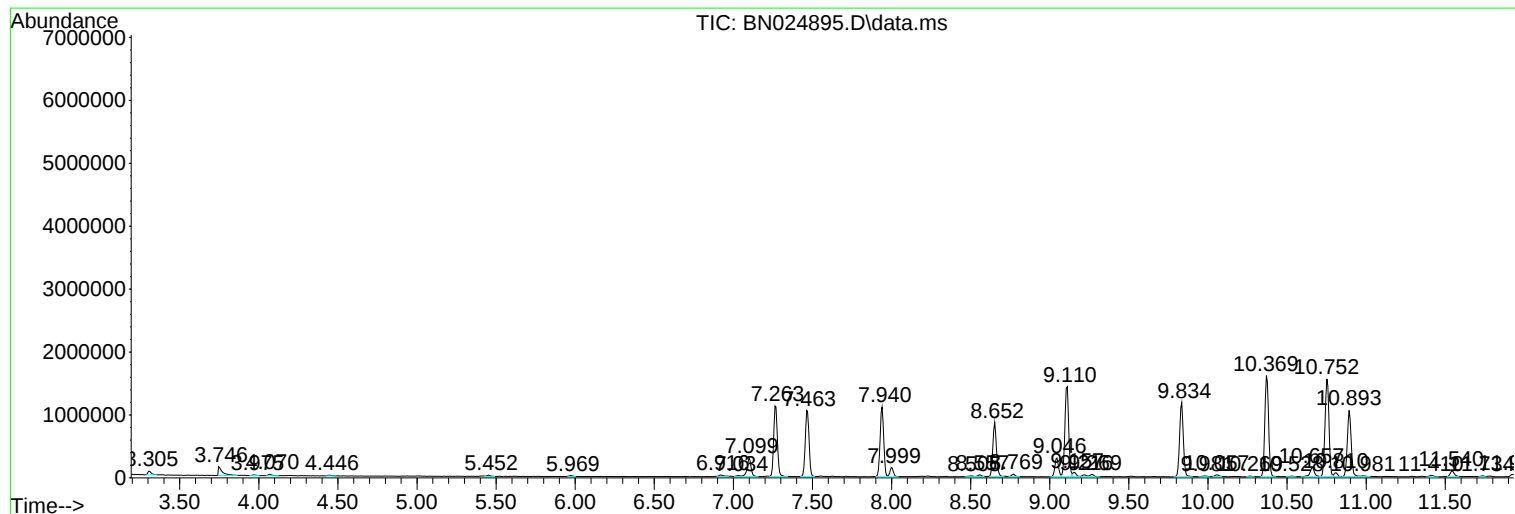
Sum of corrected areas: 93694995

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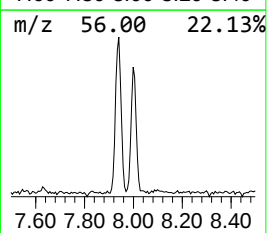
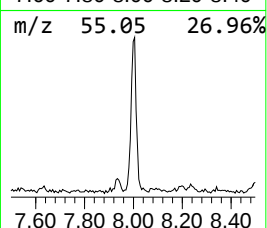
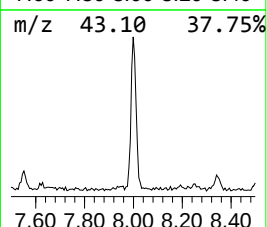
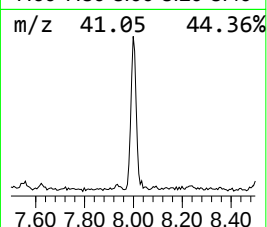
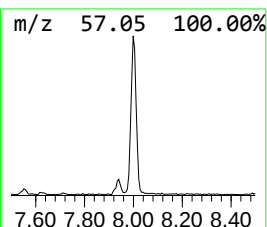
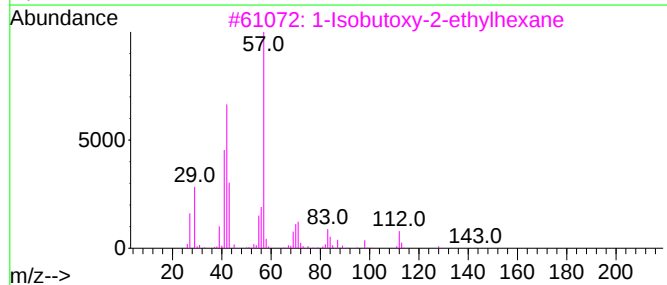
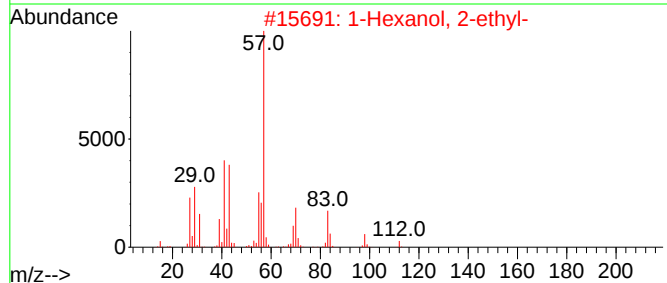
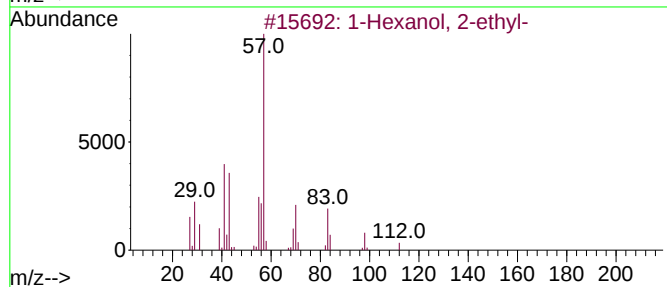
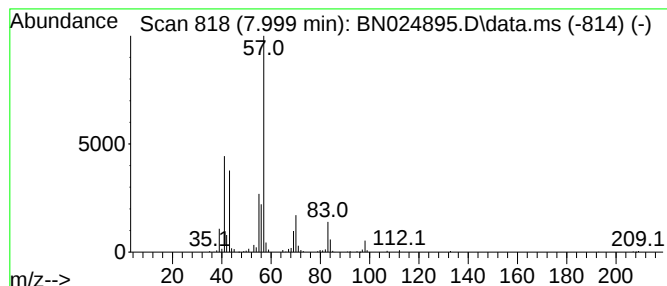
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.999	2.54 ng/ul	221745	1,4-Dichlorobenzene-d4	7.940

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	64	
3	1-Isobutoxy-2-ethylhexane		186	C12H26O	1000139-90-3	64	
4	1-Pentanol, 2-ethyl-4-methyl-		130	C8H18O	000106-67-2	59	
5	Carbonic acid, heptyl prop-1-en-...		200	C11H20O3	1000382-54-1	59	



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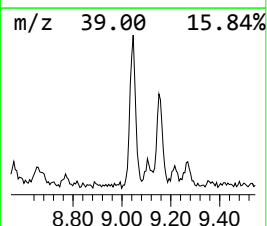
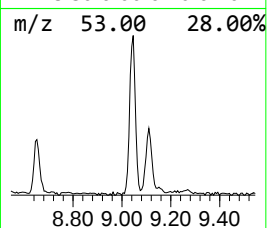
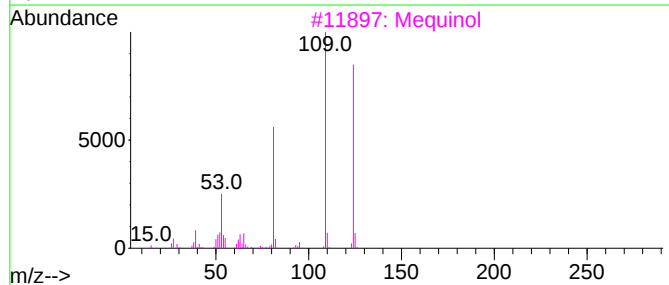
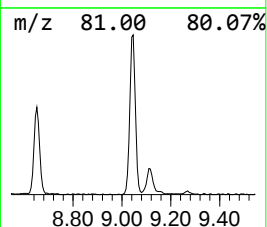
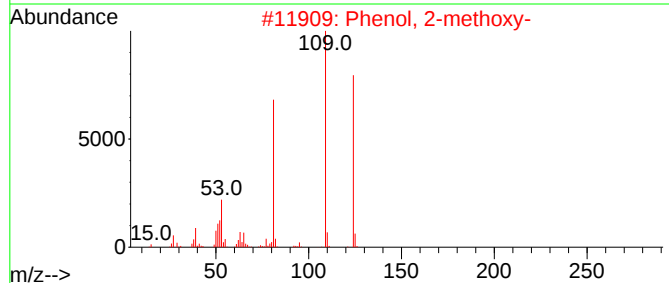
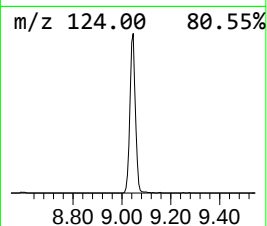
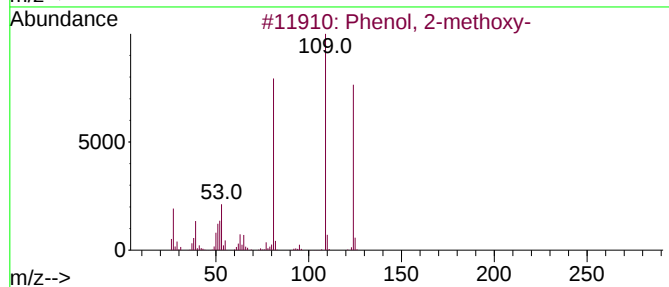
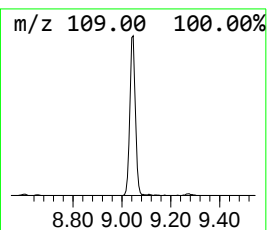
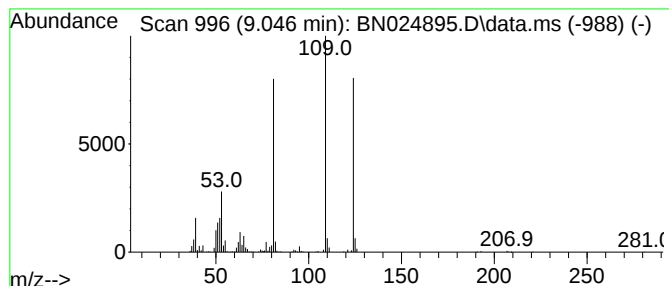
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.M
Quant Title : SVOA CALIBRATION

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.
9.046	5.58 ng/ul	487573	1,4-Dichlorobenzene-d4	7.940

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			Mequinol	124	C7H8O2	000150-76-5	92
4			Mequinol	124	C7H8O2	000150-76-5	90
5			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	90



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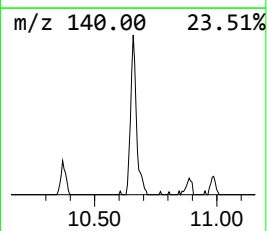
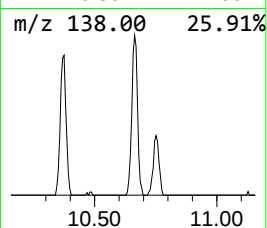
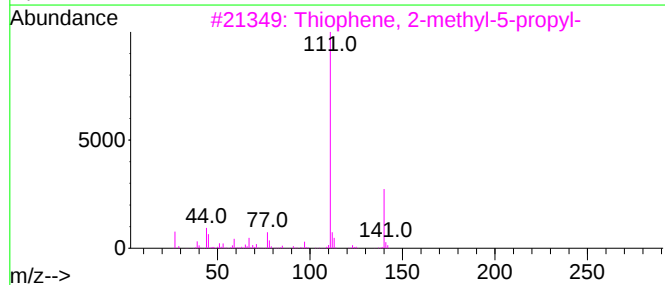
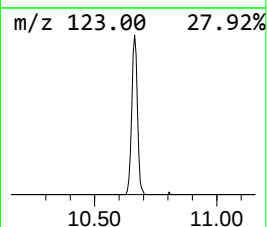
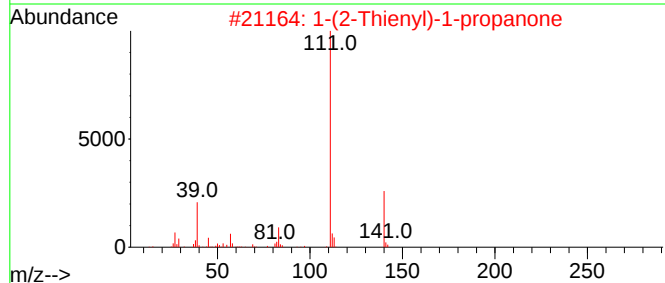
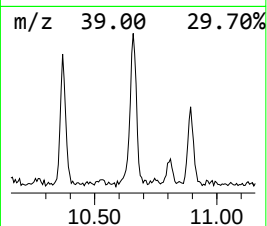
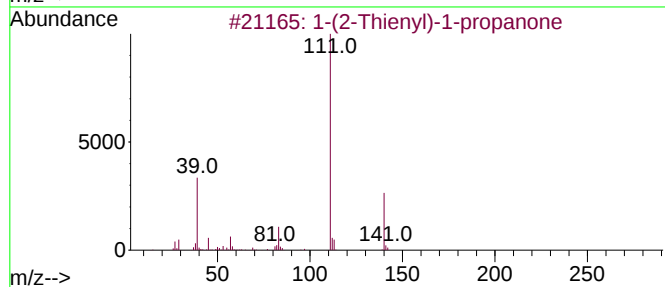
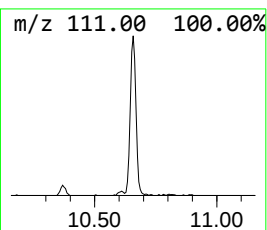
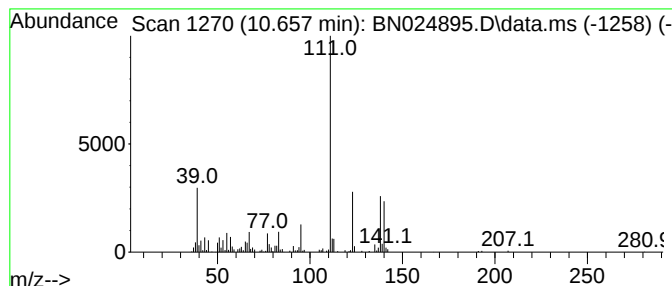
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 1-(2-Thienyl)-1-propanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.657	2.24 ng/ul	294025	Naphthalene-d8	10.752

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			Thiophene, 2-methyl-5-propyl-	140	C8H12S	033933-73-2	53
4			1-(2-Thienyl)-1-propanone	140	C7H8OS	013679-75-9	52
5			Glycine, N-(2-thienylcarbonyl)-,...	199	C8H9NO3S	1000299-60-2	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN041423\
Data File : BN024895.D
Acq On : 14 Apr 2023 13:25
Operator : CG/JU
Sample : 02252-17
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
COMF3

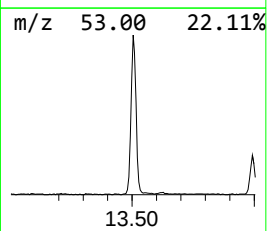
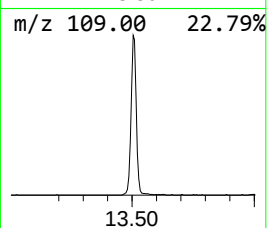
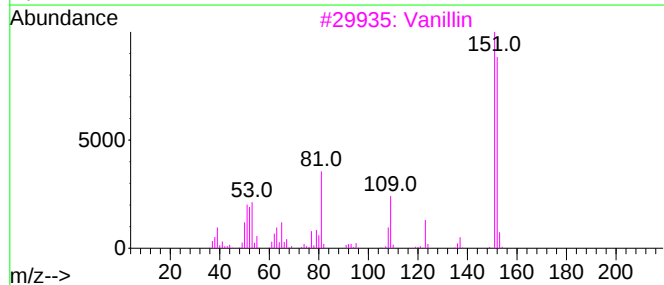
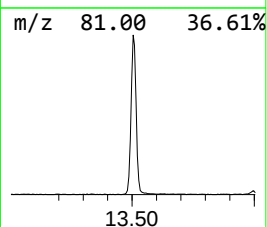
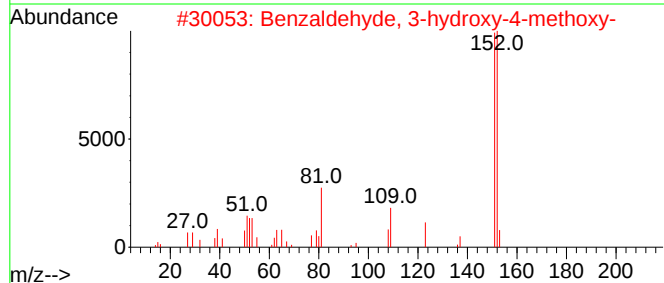
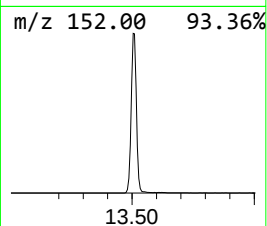
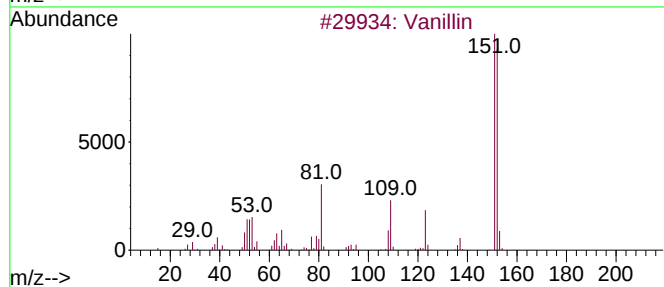
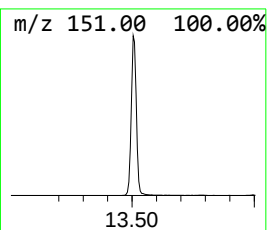
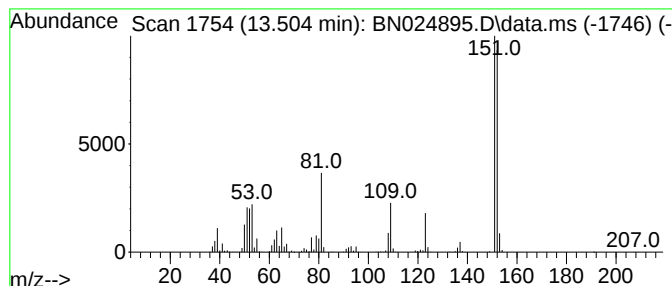
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Quant Title : SVOA CALIBRATION

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.
13.504	10.02 ng/ul	1777090	Acenaphthene-d10	14.587

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	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN041423\
Data File : BN024895.D
Acq On : 14 Apr 2023 13:25
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Sample : 02252-17
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
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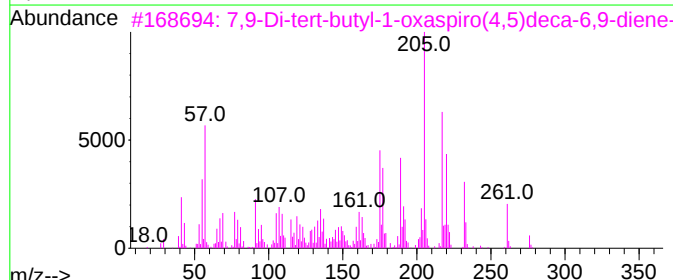
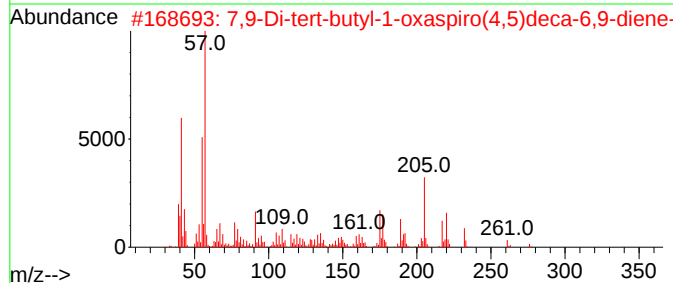
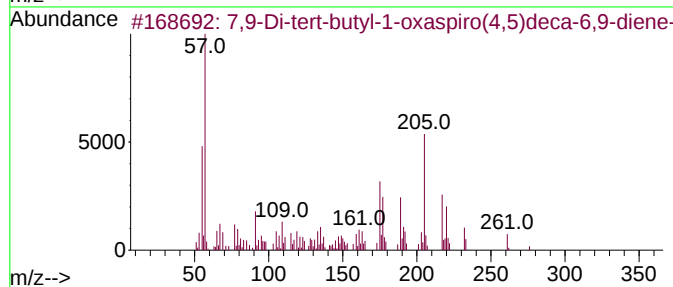
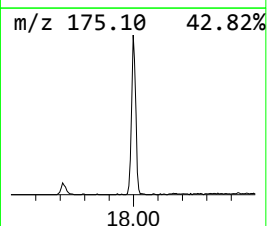
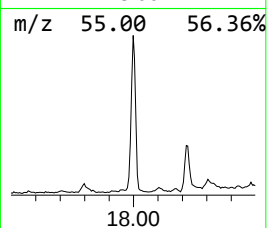
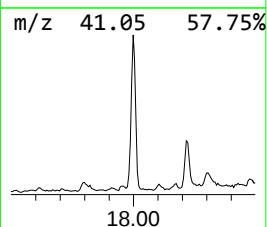
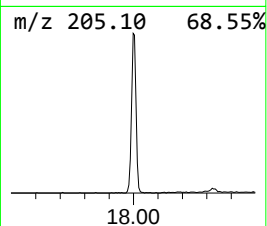
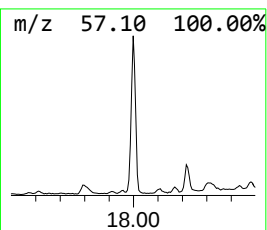
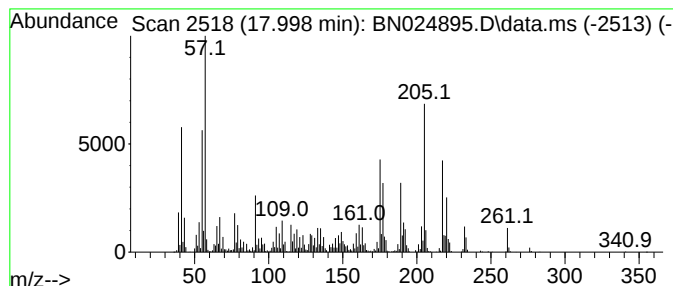
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.998	6.93 ng/ul	1450360	Phenanthrene-d10	17.334

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	86		
4	2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	48		
5	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	42		



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN041423\
Data File : BN024895.D
Acq On : 14 Apr 2023 13:25
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Sample : 02252-17
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
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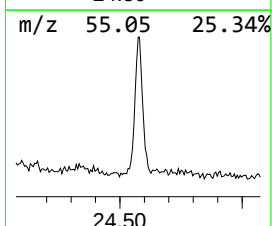
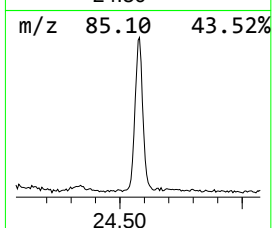
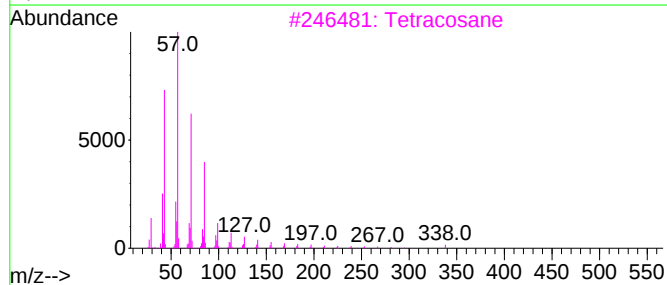
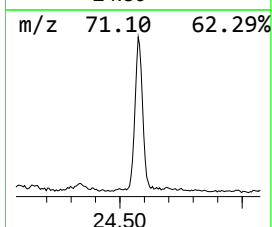
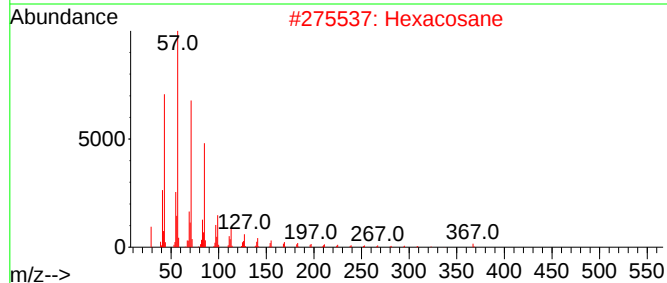
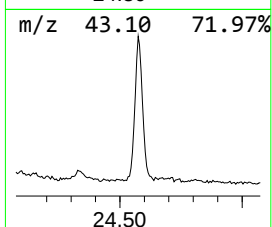
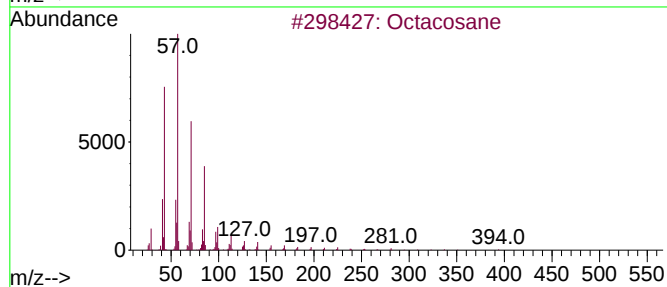
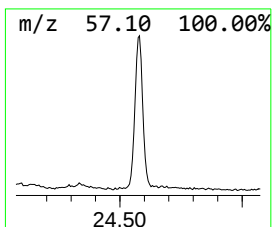
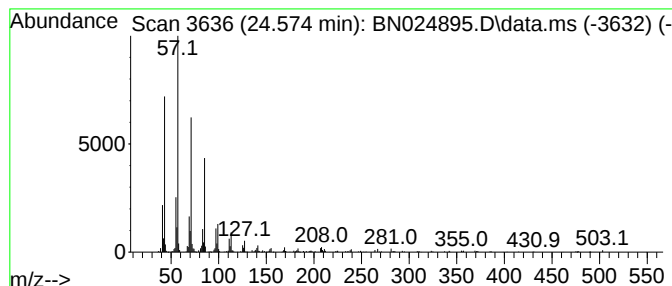
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.574	3.00 ng/ul	719137	Perylene-d12	23.968

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	90
2		Hexacosane	366	C26H54	000630-01-3	87
3		Tetracosane	338	C24H50	000646-31-1	87
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5		Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN041423\
Data File : BN024895.D
Acq On : 14 Apr 2023 13:25
Operator : CG/JU
Sample : 02252-17
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
COMF3

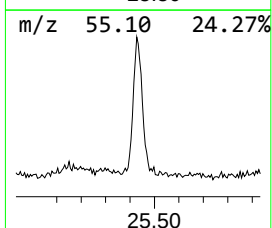
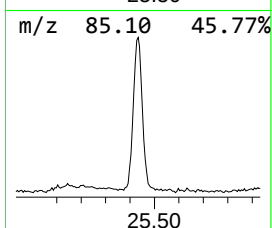
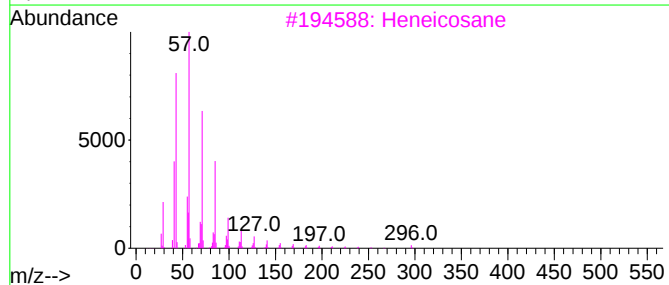
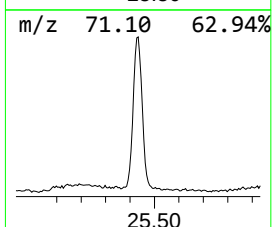
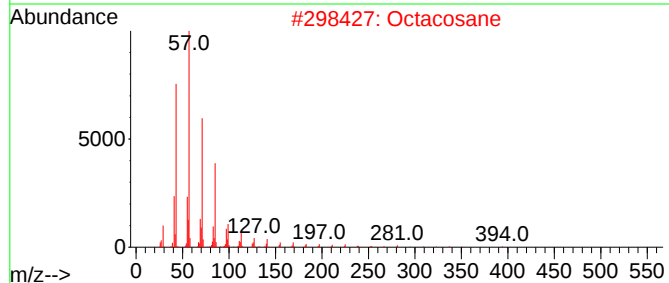
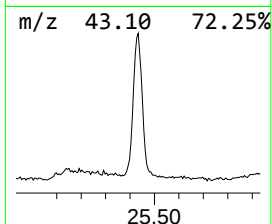
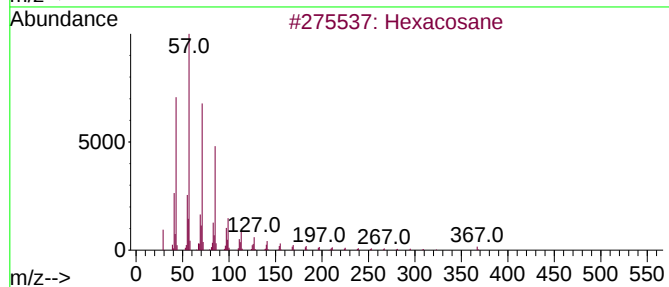
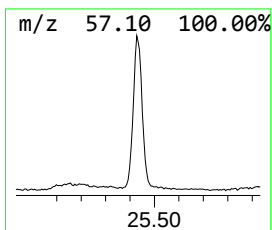
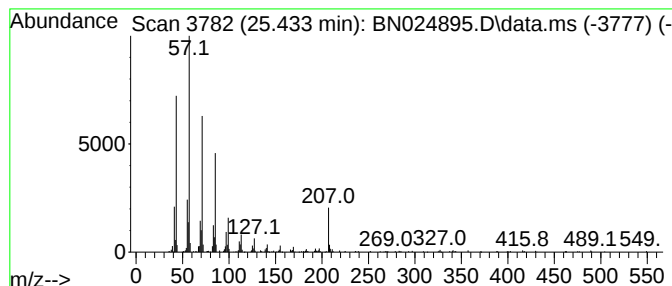
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.433	3.17 ng/ul	759774	Perylene-d12	23.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	81
2			Octacosane	394	C28H58	000630-02-4	81
3			Heneicosane	296	C21H44	000629-94-7	81
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	81
5			Octacosane	394	C28H58	000630-02-4	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN041423\
Data File : BN024895.D
Acq On : 14 Apr 2023 13:25
Operator : CG/JU
Sample : 02252-17
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
COMF3

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...	7.999	2.5	ng/ul	221745	1	7.940	1748720	20.0
Phenol, 2-methoxy-	9.046	5.6	ng/ul	487573	1	7.940	1748720	20.0
1-(2-Thienyl)-1...	10.657	2.2	ng/ul	294025	2	10.752	2620380	20.0
Vanillin	13.504	10.0	ng/ul	1777090	3	14.587	3548270	20.0
7,9-Di-tert-but...	17.998	6.9	ng/ul	1450360	4	17.334	4183440	20.0
(DEL) Alkane: S...	24.574	3.0	ng/ul	719137	6	23.968	4789580	20.0
(DEL) Alkane: S...	25.433	3.2	ng/ul	759774	6	23.968	4789580	20.0