

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN060824\
 Data File : BN031865.D
 Acq On : 08 Jun 2024 19:08
 Operator : MA/JU
 Sample : P2647-06
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 BH5T7

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-BN052924.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BN031865.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.181	29	33	42	rVB	91666	126271	1.70%	0.126%
2	3.446	74	78	89	rVB	505077	695078	9.35%	0.694%
3	3.587	100	102	114	rBV	943175	1360299	18.31%	1.358%
4	3.693	118	120	128	rVB2	24448	28832	0.39%	0.029%
5	3.905	152	156	161	rVB	35722	47653	0.64%	0.048%
6	4.569	266	269	278	rBV4	13059	23447	0.32%	0.023%
7	4.805	304	309	313	rBV2	10368	18271	0.25%	0.018%
8	4.899	320	325	331	rVB5	10716	19635	0.26%	0.020%
9	5.158	364	369	374	rVB3	8293	14123	0.19%	0.014%
10	5.769	465	473	483	rVB	55419	91767	1.23%	0.092%
11	6.275	554	559	564	rBV	10997	21879	0.29%	0.022%
12	6.687	620	629	632	rBV4	16519	34551	0.46%	0.034%
13	6.852	644	657	669	rVB	1734229	2923641	39.35%	2.919%
14	7.010	677	684	696	rVB	1371811	2162217	29.10%	2.159%
15	7.205	709	717	724	rBV	1829333	2890321	38.90%	2.886%
16	7.275	724	729	741	rVB	121945	218693	2.94%	0.218%
17	7.669	787	796	803	rBV	1470923	2298468	30.93%	2.295%
18	7.740	803	808	814	rVB2	50940	85411	1.15%	0.085%
19	8.381	908	917	931	rBV	2264743	3692619	49.69%	3.686%
20	8.828	985	993	1001	rBV	1701066	2798978	37.67%	2.794%
21	8.952	1008	1014	1016	rBV3	9413	15482	0.21%	0.015%
22	8.987	1016	1020	1027	rVB7	18410	31696	0.43%	0.032%
23	9.216	1054	1059	1064	rBV	12700	23179	0.31%	0.023%
24	9.393	1079	1089	1096	rBV	290411	451462	6.08%	0.451%
25	9.546	1107	1115	1127	rBV	1386707	2360391	31.77%	2.356%
26	9.781	1151	1155	1160	rBV3	14896	28140	0.38%	0.028%
27	10.081	1191	1206	1222	rBV	2186969	3721151	50.08%	3.715%
28	10.234	1227	1232	1242	rBV	128946	226167	3.04%	0.226%
29	10.451	1261	1269	1277	rBV	2039710	3486016	46.91%	3.480%
30	10.599	1283	1294	1313	rBV	1927818	3379764	45.48%	3.374%
31	10.963	1349	1356	1357	rBV7	7754	15321	0.21%	0.015%
32	10.999	1357	1362	1371	rVB2	120233	192086	2.59%	0.192%
33	11.199	1388	1396	1416	rBV	484105	942476	12.68%	0.941%
34	11.469	1436	1442	1447	rVV3	11520	20064	0.27%	0.020%
35	11.881	1504	1512	1517	rBV4	13258	23337	0.31%	0.023%
36	11.957	1521	1525	1530	rBV2	12862	20716	0.28%	0.021%

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Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN052924.MA.M
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37	12.046	1535	1540	1548	rVV2	41233	78997	1.06%	0.079%
38	12.122	1548	1553	1558	rVB2	20940	34912	0.47%	0.035%
39	12.263	1571	1577	1582	rBV9	6921	16801	0.23%	0.017%
40	12.340	1586	1590	1597	rVV	25050	41901	0.56%	0.042%
41	12.916	1681	1688	1696	rVB	6122	16159	0.22%	0.016%
42	13.134	1721	1725	1733	rVB2	27073	44095	0.59%	0.044%
43	13.281	1746	1750	1755	rVB4	11845	18574	0.25%	0.019%
44	13.492	1778	1786	1797	rBV9	21747	62174	0.84%	0.062%
45	13.587	1797	1802	1805	rVV6	7623	14721	0.20%	0.015%
46	13.634	1805	1810	1814	rVV2	30039	53713	0.72%	0.054%
47	13.687	1814	1819	1820	rVV4	23124	32865	0.44%	0.033%
48	13.728	1820	1826	1834	rVV	3373741	4903040	65.98%	4.895%
49	13.792	1834	1837	1841	rVV4	19461	30658	0.41%	0.031%
50	13.840	1841	1845	1847	rVV5	9159	15714	0.21%	0.016%
51	13.869	1847	1850	1854	rVV	16378	22293	0.30%	0.022%
52	14.010	1867	1874	1884	rVB	3956939	6407833	86.23%	6.397%
53	14.216	1904	1909	1915	rVB	24416	36734	0.49%	0.037%
54	14.316	1915	1926	1932	rBV	2946707	4458307	60.00%	4.451%
55	14.534	1956	1963	1980	rVV	1678500	2849781	38.35%	2.845%
56	14.681	1985	1988	1991	rBV2	15502	20270	0.27%	0.020%
57	14.716	1991	1994	1996	rBV	13986	15686	0.21%	0.016%
58	14.792	2003	2007	2010	rVV2	11961	15735	0.21%	0.016%
59	14.834	2010	2014	2021	rVB10	12972	27763	0.37%	0.028%
60	14.934	2027	2031	2035	rBV5	10288	17384	0.23%	0.017%
61	14.987	2035	2040	2045	rVB5	14887	24241	0.33%	0.024%
62	15.104	2055	2060	2064	rBV4	21948	41083	0.55%	0.041%
63	15.169	2068	2071	2076	rVB	23487	30282	0.41%	0.030%
64	15.310	2088	2095	2102	rBV	5032909	7430780	100.00%	7.418%
65	15.439	2111	2117	2130	rVV	961538	1375156	18.51%	1.373%
66	15.551	2132	2136	2144	rVB4	30559	68438	0.92%	0.068%
67	15.657	2149	2154	2161	rVB7	22675	45427	0.61%	0.045%
68	15.810	2178	2180	2185	rVB6	10179	14528	0.20%	0.015%
69	15.869	2185	2190	2199	rVB9	18783	42570	0.57%	0.042%
70	16.034	2213	2218	2225	rBV6	43381	107697	1.45%	0.108%
71	16.086	2225	2227	2233	rVB6	10892	15860	0.21%	0.016%
72	16.204	2245	2247	2254	rVB7	10771	16532	0.22%	0.017%
73	16.475	2289	2293	2296	rBV6	12284	19587	0.26%	0.020%
74	16.722	2331	2335	2342	rBV4	18000	36749	0.49%	0.037%
75	16.828	2349	2353	2355	rBV	22576	27885	0.38%	0.028%
76	16.986	2377	2380	2386	rVB8	16487	21577	0.29%	0.022%

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77	17.063	2386	2393	2398	rBV	3158425	4583372	61.68%	4.576%
78	17.104	2398	2400	2404	rVV	134858	160731	2.16%	0.160%
79	17.163	2404	2410	2419	rVB2	4488182	6581871	88.58%	6.571%
80	17.328	2434	2438	2451	rVB5	48187	130913	1.76%	0.131%
81	17.563	2474	2478	2482	rBV2	29360	43403	0.58%	0.043%
82	17.739	2504	2508	2512	rVB	68141	85039	1.14%	0.085%
83	17.963	2538	2546	2562	rBV3	827943	1523510	20.50%	1.521%
84	18.128	2570	2574	2578	rBV3	38581	58948	0.79%	0.059%
85	18.257	2593	2596	2598	rBV2	31880	38170	0.51%	0.038%
86	18.292	2598	2602	2614	rVB3	146102	264170	3.56%	0.264%
87	18.445	2625	2628	2632	rVB3	35514	48931	0.66%	0.049%
88	18.863	2696	2699	2702	rBV2	26973	35379	0.48%	0.035%
89	19.022	2723	2726	2728	rBV2	43625	58303	0.78%	0.058%
90	19.051	2728	2731	2734	rVB	82280	101192	1.36%	0.101%
91	19.098	2735	2739	2740	rBV	68633	79437	1.07%	0.079%
92	19.127	2740	2744	2751	rVB	296828	405342	5.45%	0.405%
93	19.251	2761	2765	2773	rBV2	174468	291667	3.93%	0.291%
94	19.463	2795	2801	2814	rBV2	4681294	6883406	92.63%	6.872%
95	20.551	2984	2986	2990	rVB2	104262	108902	1.47%	0.109%
96	20.986	3056	3060	3067	rBV	921240	1227043	16.51%	1.225%
97	21.304	3108	3114	3119	rBV2	2198075	3556365	47.86%	3.550%
98	22.663	3340	3345	3353	rBV4	601314	1230911	16.57%	1.229%
99	24.039	3572	3579	3588	rVB3	2307457	5649857	76.03%	5.640%
100	24.245	3606	3614	3624	rVB	1580377	3975484	53.50%	3.969%

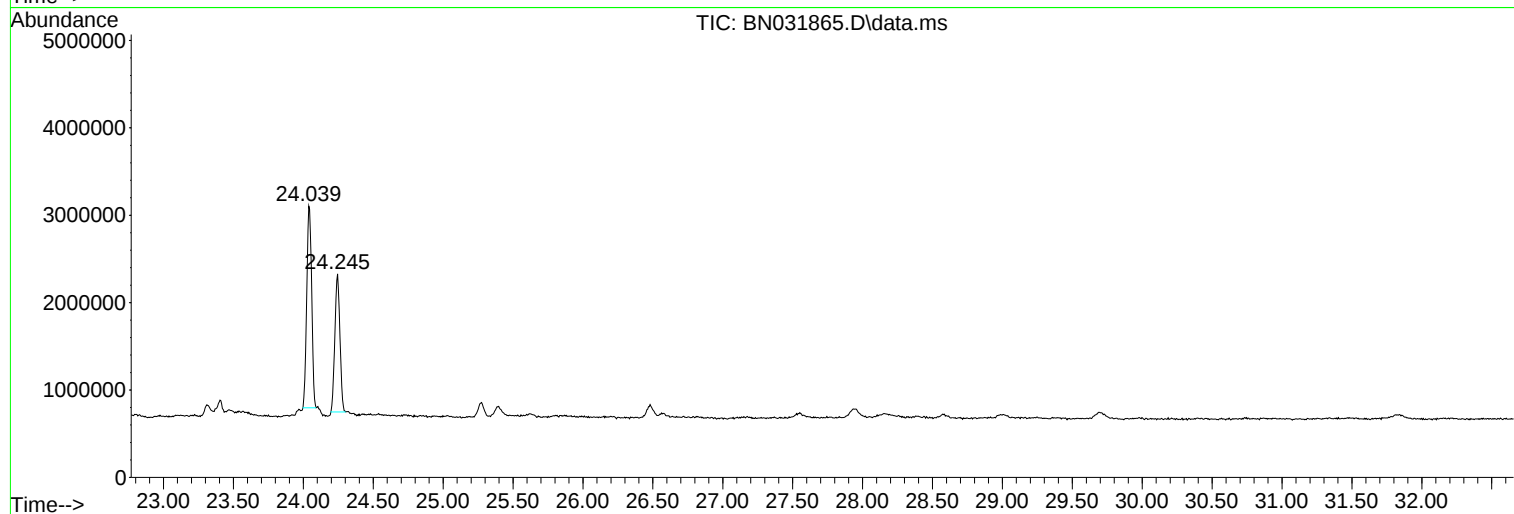
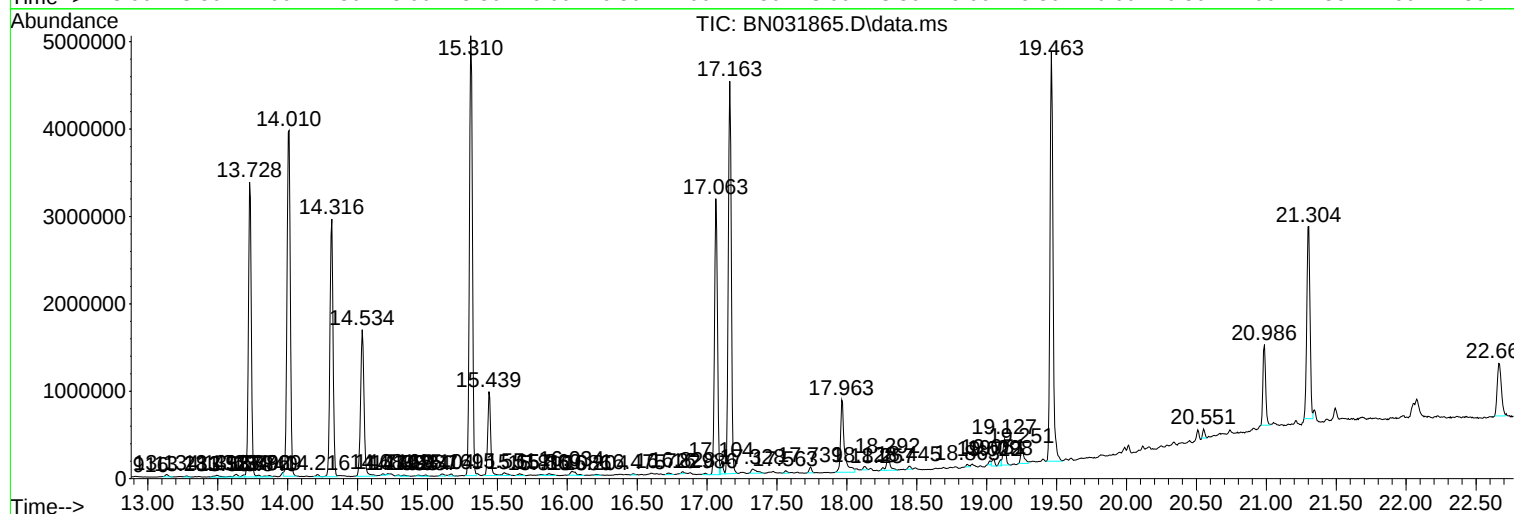
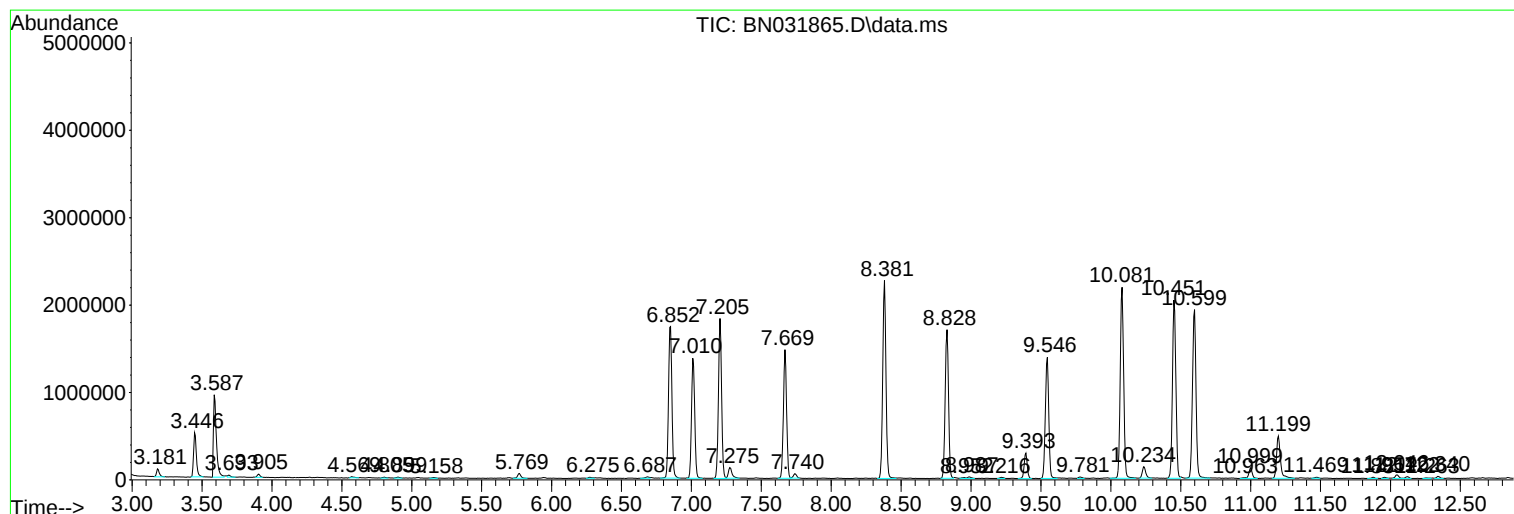
Sum of corrected areas: 100166450

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ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_N
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN052924.MA.M
Quant Title : SVOA CALIBRATION

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



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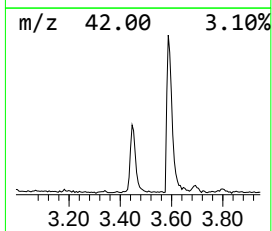
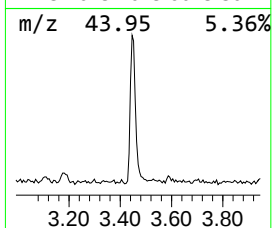
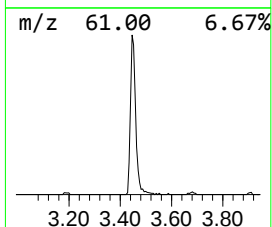
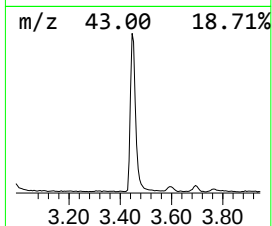
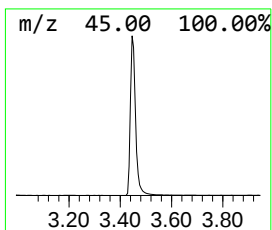
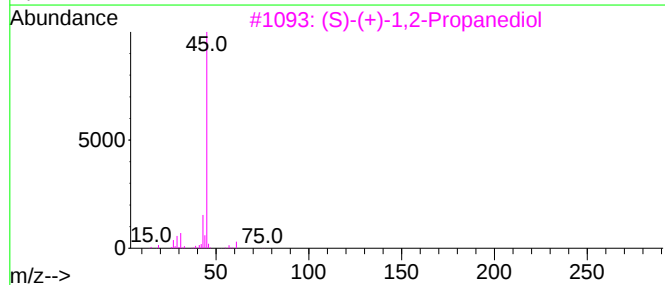
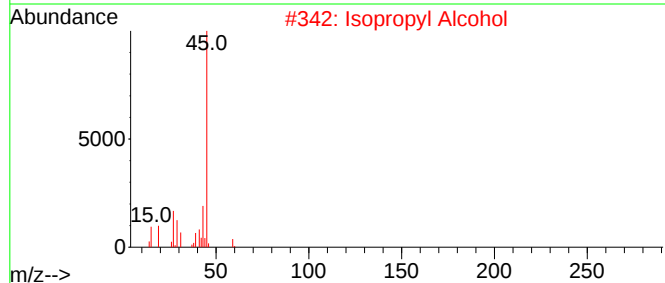
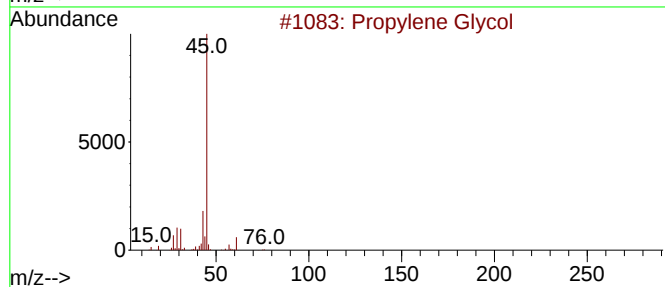
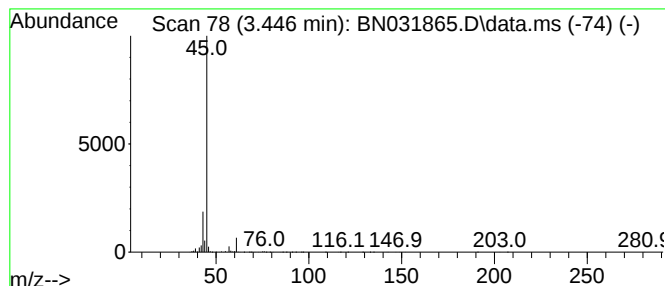
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN052924.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.446	6.05 ng/ul	695078	1,4-Dichlorobenzene-d4	7.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	90
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	37



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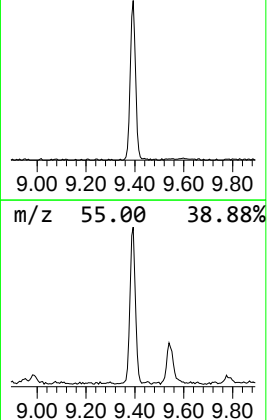
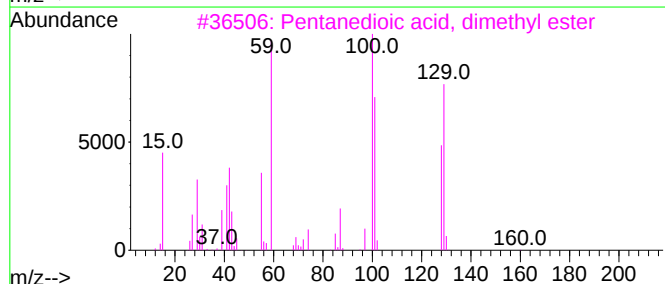
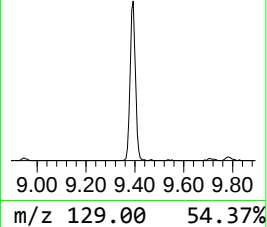
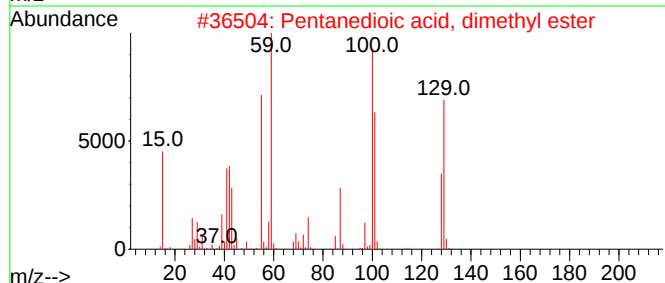
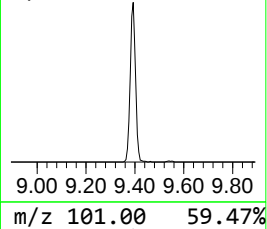
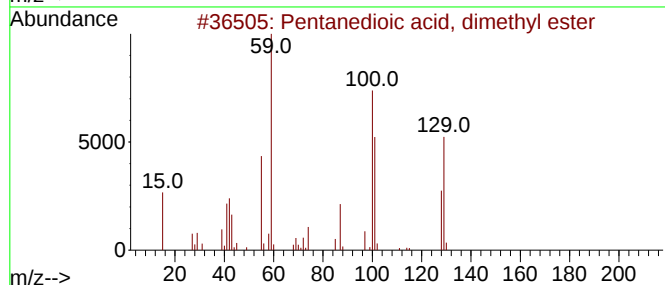
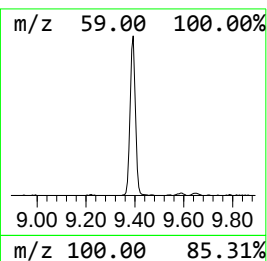
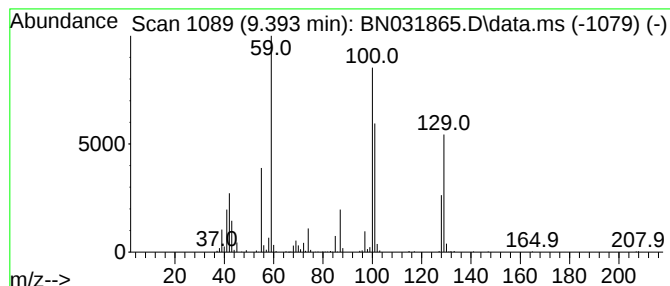
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN052924.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Pentanedioic acid, dimethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.393	2.59 ng/ul	451462	Naphthalene-d8	10.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	91
2			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	83
3			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	83
4			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	83
5			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	64



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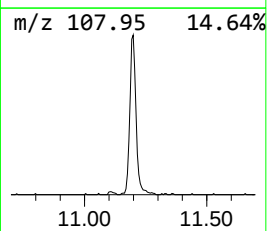
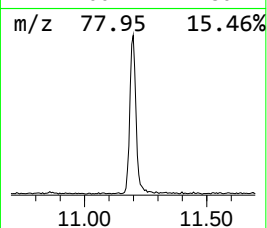
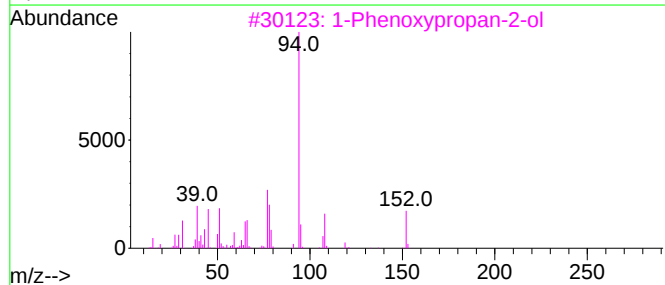
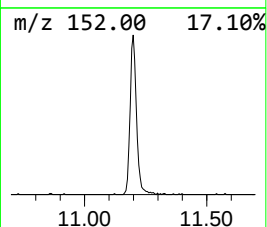
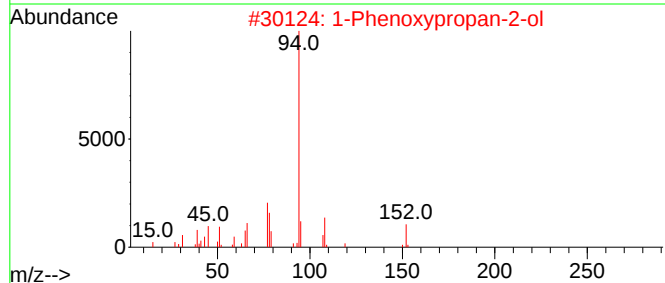
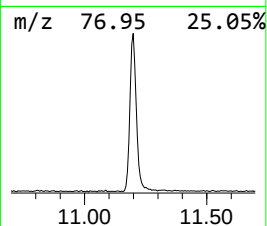
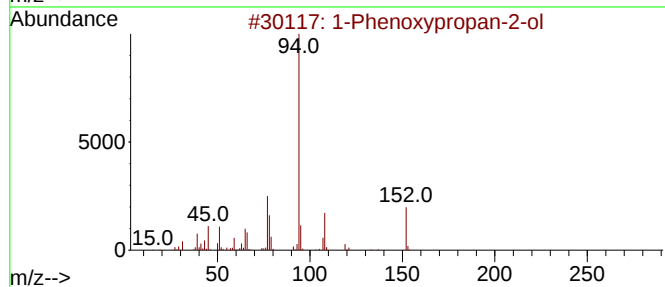
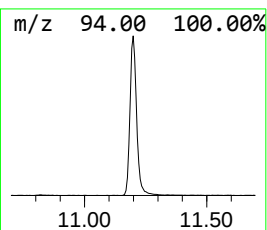
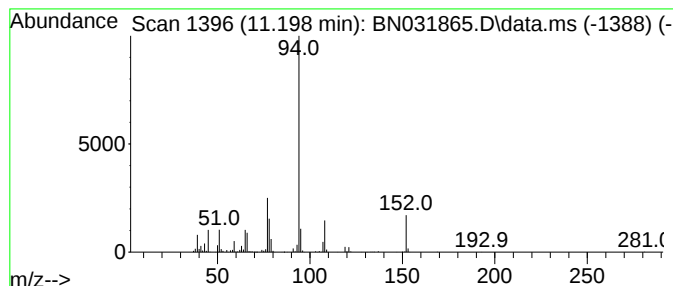
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN052924.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.198	5.41 ng/ul	942476	Naphthalene-d8	10.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
3			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
4			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	83
5			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN060824\
Data File : BN031865.D
Acq On : 08 Jun 2024 19:08
Operator : MA/JU
Sample : P2647-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
BH5T7

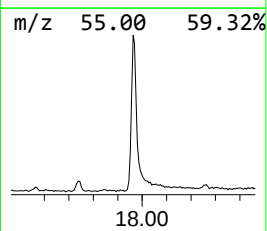
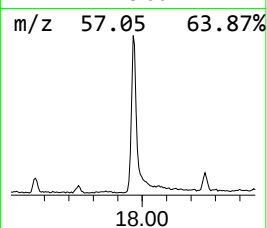
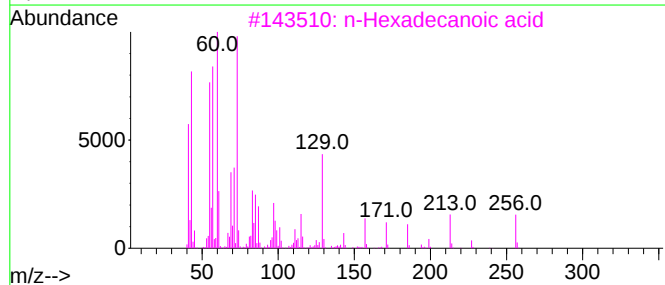
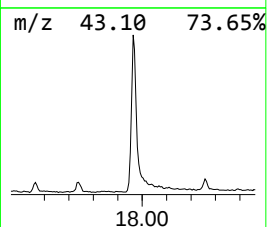
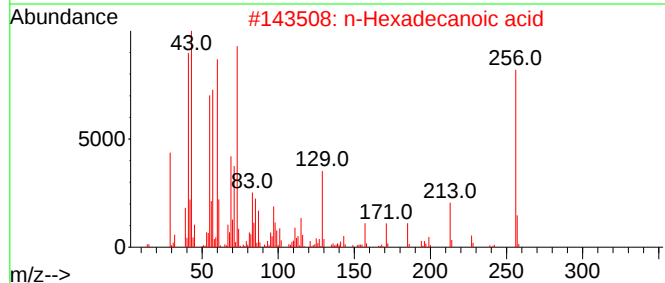
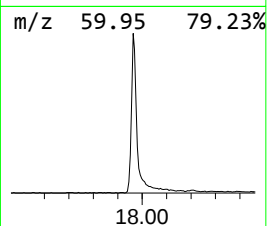
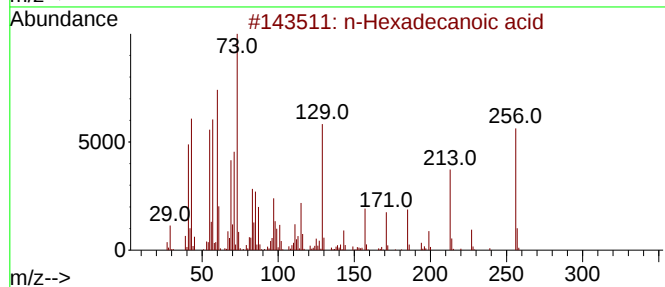
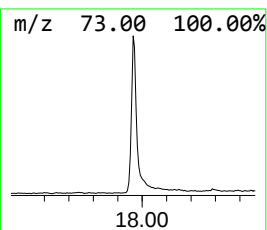
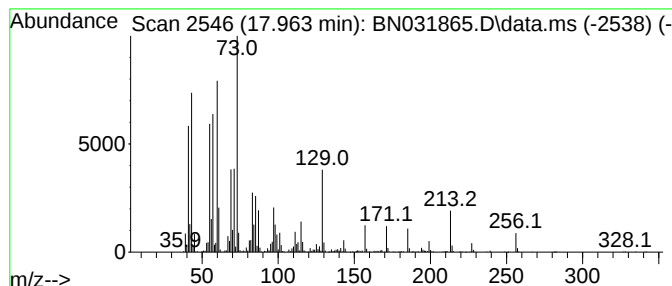
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.963	6.65 ng/ul	1523510	Phenanthrene-d10	17.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
5			Octadecanoic acid	284	C18H36O2	000057-11-4	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN060824\
Data File : BN031865.D
Acq On : 08 Jun 2024 19:08
Operator : MA/JU
Sample : P2647-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

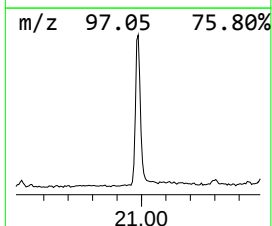
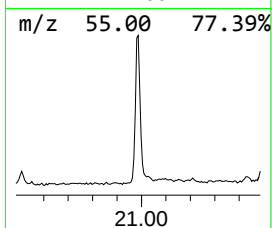
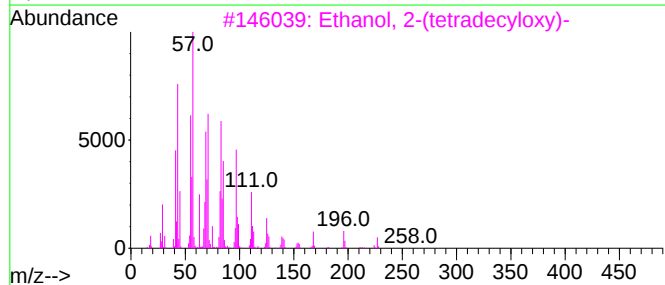
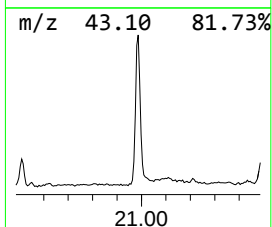
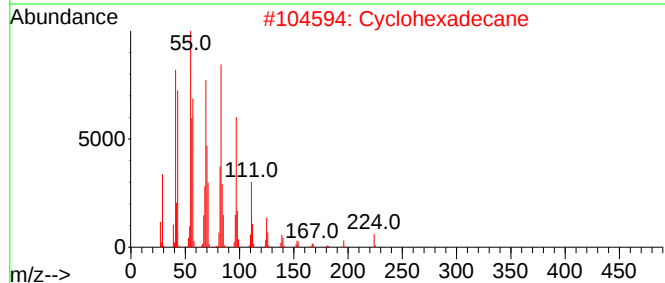
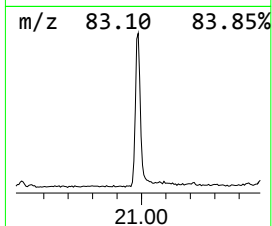
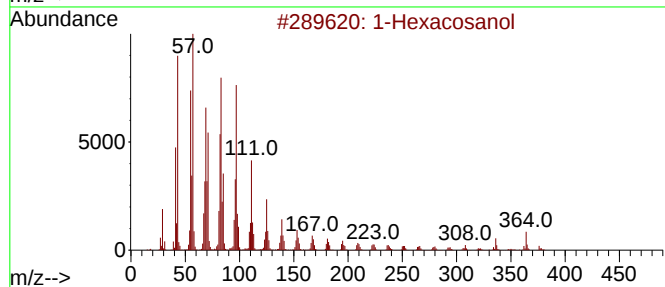
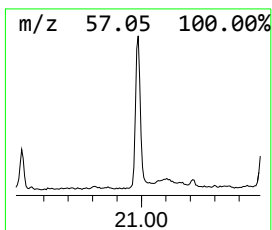
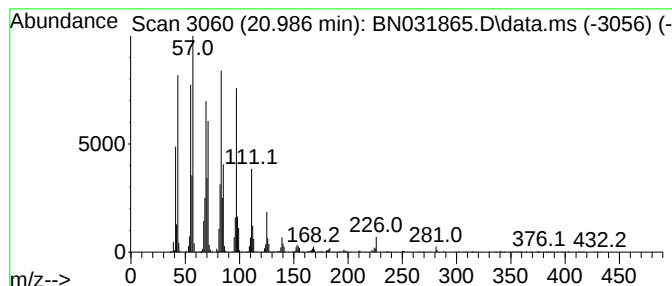
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 1-Hexacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.986	6.90 ng/ul	1227040	Chrysene-d12	21.304	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol	382	C26H54O	000506-52-5	94
2	Cyclohexadecane	224	C16H32	000295-65-8	94
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	1-Heptacosanol	396	C27H56O	002004-39-9	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN060824\
Data File : BN031865.D
Acq On : 08 Jun 2024 19:08
Operator : MA/JU
Sample : P2647-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
BH5T7

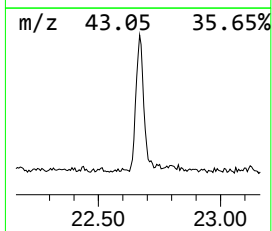
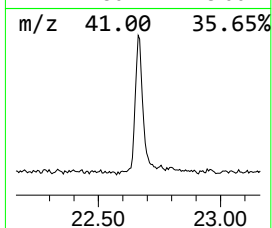
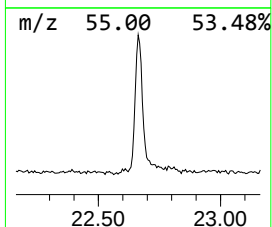
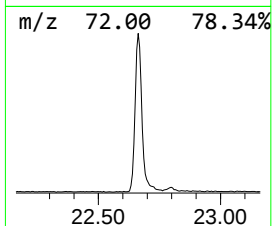
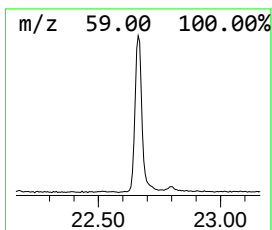
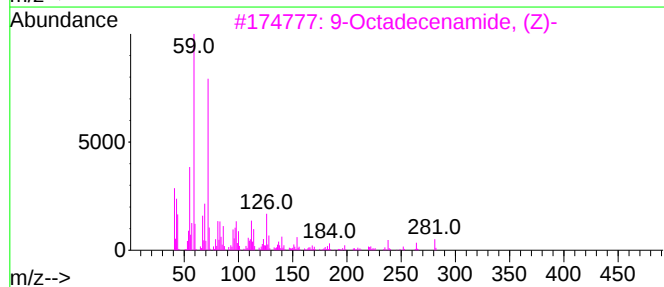
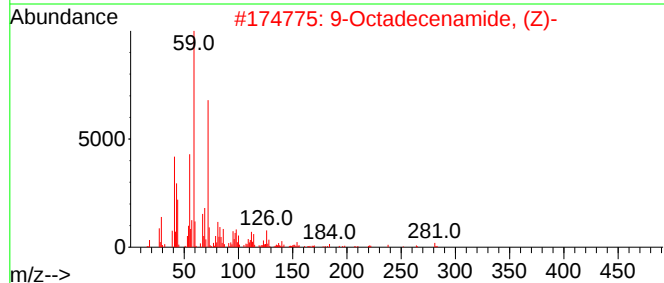
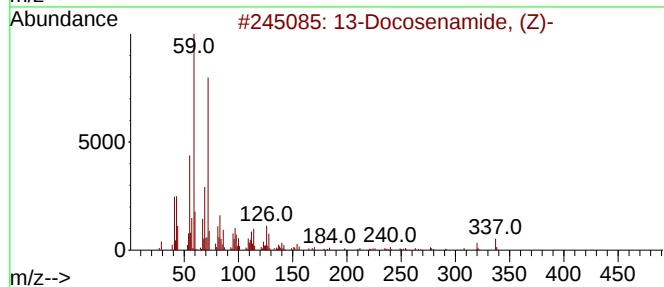
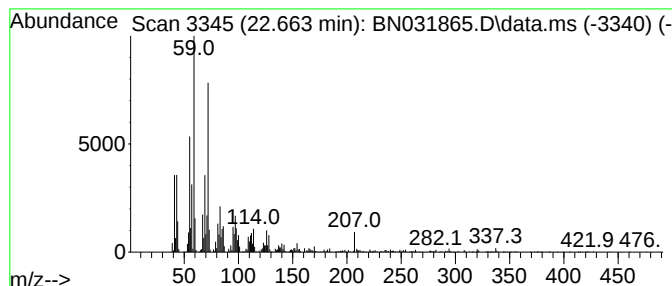
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.663	6.92 ng/ul	1230910	Chrysene-d12	21.304

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	99
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
3		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	72
4		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	64
5		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN060824\
Data File : BN031865.D
Acq On : 08 Jun 2024 19:08
Operator : MA/JU
Sample : P2647-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
BH5T7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN052924.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
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Pentanedioic ac...	9.393	2.6	ng/ul	451462	2	10.451	3486020	20.0
1-Phenoxypropan...	11.198	5.4	ng/ul	942476	2	10.451	3486020	20.0
n-Hexadecanoic ...	17.963	6.7	ng/ul	1523510	4	17.063	4583370	20.0
1-Hexacosanol	20.986	6.9	ng/ul	1227040	5	21.304	3556370	20.0
13-Docosenamide...	22.663	6.9	ng/ul	1230910	5	21.304	3556370	20.0