LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081524\
Data File : BN033395.D
Acq On : 15 Aug 2024 11:42
Operator : MA/JU
Sample : P3481-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E0AE2

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-BN081424.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BN033395.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.158	25	29	43	rVB	89182	139225	1.26%	0.119%
2	3.411	68	72	90	rVB	204905	305901	2.77%	0.261%
3	3.546	90	95	117	rVB	828694	1331917	12.07%	1.136%
4	3.864	146	149	156	rVB	18727	29686	0.27%	0.025%
5	4.746	292	299	307	rBV4	9094	17928	0.16%	0.015%
6	5.693	454	460	466	rBV	29288	41838	0.38%	0.036%
7	6.516	594	600	606	rBV8	8594	15444	0.14%	0.013%
8	6.575	606	610	621	rBV6	10183	22213	0.20%	0.019%
9	6.752	631	640	654	rVB	1856198	2933501	26.59%	2.503%
10	6.869	654	660	662	rVV	31589	45165	0.41%	0.039%
11	6.916	662	668	680	rVB	1514081	2264732	20.52%	1.932%
12	7.105	693	700	709	rBV	1817013	2830733	25.65%	2.415%
13	7.181	709	713	728	rVB	66772	132160	1.20%	0.113%
14	7.375	740	746	753	rVB4	6716	14489	0.13%	0.012%
15	7.569	771	779	786	rBV	1572228	2457579	22.27%	2.097%
16	7.646	788	792	796	rVV2	23458	33874	0.31%	0.029%
17	7.922	834	839	847	rVB8	6483	13625	0.12%	0.012%
18	8.269	889	898	911	rBV	2390844	3772477	34.19%	3.219%
19	8.710	964	973	980	rBV	1699871	2779425	25.19%	2.371%
20	8.893	998	1004	1008	rBV7	7318	12576	0.11%	0.011%
21	9.187	1051	1054	1058	rVB5	8998	12845	0.12%	0.011%
22	9.287	1066	1071	1080	rVB	154554	228405	2.07%	0.195%
23	9.422	1086	1094	1105	rBV	1337910	2110613	19.13%	1.801%
24	9.663	1130	1135	1144	rVB	5590	14873	0.13%	0.013%
25	9.957	1177	1185	1195	rBV	2337886	3763401	34.11%	3.211%
26	10.134	1212	1215	1222	rVB6	7621	14499	0.13%	0.012%
27	10.334	1241	1249	1256	rBV	2365620	3869966	35.07%	3.302%
28	10.469	1264	1272	1282	rBV	1363641	2258780	20.47%	1.927%
29	10.810	1325	1330	1334	rBV6	8300	17298	0.16%	0.015%
30	10.893	1337	1344	1351	rVB	99679	146630	1.33%	0.125%
31	11.081	1369	1376	1383	rBV	544345	871221	7.90%	0.743%
32	11.240	1399	1403	1407	rBV3	8468	15108	0.14%	0.013%
33	11.851	1503	1507	1511	rVB4	6157	11181	0.10%	0.010%
34	11.928	1514	1520	1526	rBV	49441	81008	0.73%	0.069%
35	12.210	1561	1568	1573	rBV4	5512	13540	0.12%	0.012%
36	13.063	1707	1713	1717	rBV6	9485	15579	0.14%	0.013%

LSC Area Percent Report

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Sample : P3481-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E0AE2

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-BN081424.MA.M
Title : SVOA CALIBRATION

37	13.628	1802	1809	1818	rBV	4111808	5620079	50.93%	4.795%
38	13.898	1847	1855	1864	rBV2	4554393	6895640	62.49%	5.883%
39	14.151	1893	1898	1901	rBV2	9966	14168	0.13%	0.012%
40	14.210	1901	1908	1916	rVV	3554101	5240189	47.49%	4.471%
41	14.410	1931	1942	1946	rBV	1733449	2465019	22.34%	2.103%
42	14.445	1946	1948	1949	rVV	226484	227028	2.06%	0.194%
43	14.463	1949	1951	1960	rVB	250477	314240	2.85%	0.268%
44	14.640	1977	1981	1987	rVB8	15646	30921	0.28%	0.026%
45	14.740	1991	1998	2010	rBV	34661	74382	0.67%	0.063%
46	15.045	2046	2050	2054	rBV3	15045	22274	0.20%	0.019%
47	15.110	2057	2061	2064	rVB3	13496	15742	0.14%	0.013%
48	15.210	2070	2078	2090	rBV	5682893	8421947	76.32%	7.186%
49	15.322	2091	2097	2109	rVV	1209286	1621527	14.70%	1.384%
50	15.404	2109	2111	2114	rVV2	17130	21344	0.19%	0.018%
51	15.445	2114	2118	2122	rVB3	28051	45058	0.41%	0.038%
52	15.663	2152	2155	2162	rBV7	8714	14082	0.13%	0.012%
53	15.781	2170	2175	2182	rBV8	10686	23104	0.21%	0.020%
54	15.969	2203	2207	2210	rBV	21552	33253	0.30%	0.028%
55	16.392	2274	2279	2283	rBV7	9927	16544	0.15%	0.014%
56	16.551	2303	2306	2309	rBV3	14936	17118	0.16%	0.015%
57	16.639	2318	2321	2327	rVB7	8677	11590	0.11%	0.010%
58	16.710	2329	2333	2337	rBV5	13951	27501	0.25%	0.023%
59	16.763	2340	2342	2346	rVB3	12847	15429	0.14%	0.013%
60	16.957	2368	2375	2381	rBV	4482063	6250635	56.65%	5.333%
61	17.057	2385	2392	2403	rBV	6760674	9349507	84.73%	7.977%
62	17.163	2406	2410	2414	rBV3	43249	54834	0.50%	0.047%
63	17.345	2436	2441	2451	rVB2	50649	90621	0.82%	0.077%
64	17.675	2490	2497	2500	rBV4	30774	47786	0.43%	0.041%
65	17.892	2529	2534	2543	rBV	618097	877758	7.95%	0.749%
66	18.181	2579	2583	2590	rVB6	23075	44082	0.40%	0.038%
67	18.334	2606	2609	2614	rBV7	11530	17360	0.16%	0.015%
68	18.563	2645	2648	2651	rBV5	11962	13259	0.12%	0.011%
69	18.922	2705	2709	2715	rVB2	99675	130131	1.18%	0.111%
70	18.992	2716	2721	2724	rBV	114786	164300	1.49%	0.140%
71	19.028	2724	2727	2730	rVV2	44616	57782	0.52%	0.049%
72	19.063	2730	2733	2737	rVB6	16069	21134	0.19%	0.018%
73	19.181	2749	2753	2760	rBV2	174812	253110	2.29%	0.216%
74	19.357	2777	2783	2790	rBV	8044135	11034379	100.00%	9.415%
75	19.416	2790	2793	2798	rVV	561144	721304	6.54%	0.615%
76	20.922	3045	3049	3056	rBV	587068	827889	7.50%	0.706%

LSC Area Percent Report

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Operator : MA/JU
Sample : P3481-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E0AE2

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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Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN081424.MA.M
Title : SVOA CALIBRATION

77	21.192	3089	3095	3104	rBV	4779336	6737199	61.06%	5.748%
78	21.992	3228	3231	3240	rVB3	74264	118172	1.07%	0.101%
79	23.316	3451	3456	3472	rVB	158861	381862	3.46%	0.326%
80	23.833	3534	3544	3562	rVB	4311647	9995935	90.59%	8.529%
81	24.021	3567	3576	3588	rVB	2679981	6186871	56.07%	5.279%

Sum of corrected areas: 117203524

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Acq On : 15 Aug 2024 11:42
Operator : MA/JU
Sample : P3481-02
Misc :
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Instrument :
BNA_N
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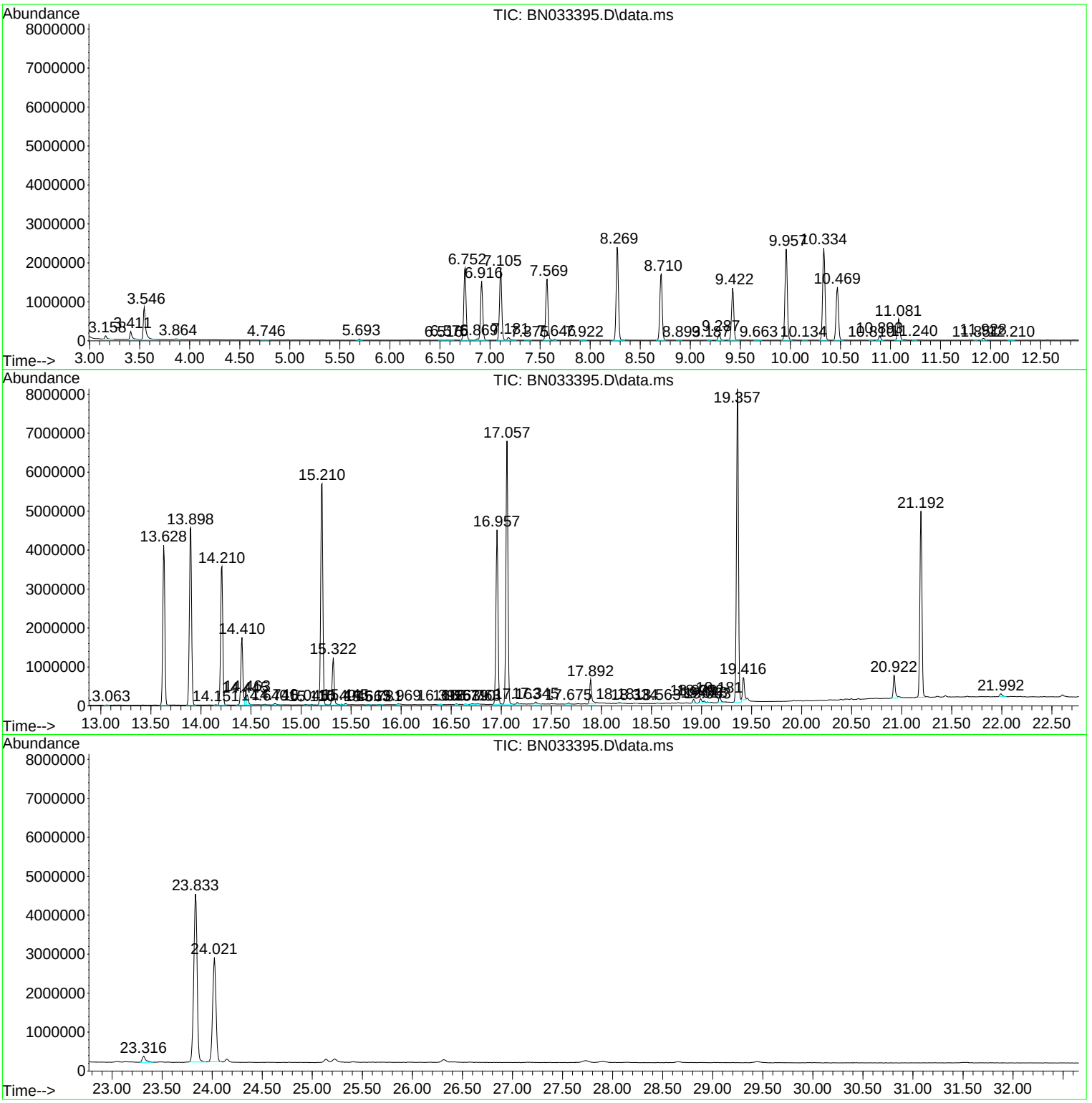
E0AE2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN081424.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081524\
Data File : BN033395.D
Acq On : 15 Aug 2024 11:42
Operator : MA/JU
Sample : P3481-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E0AE2

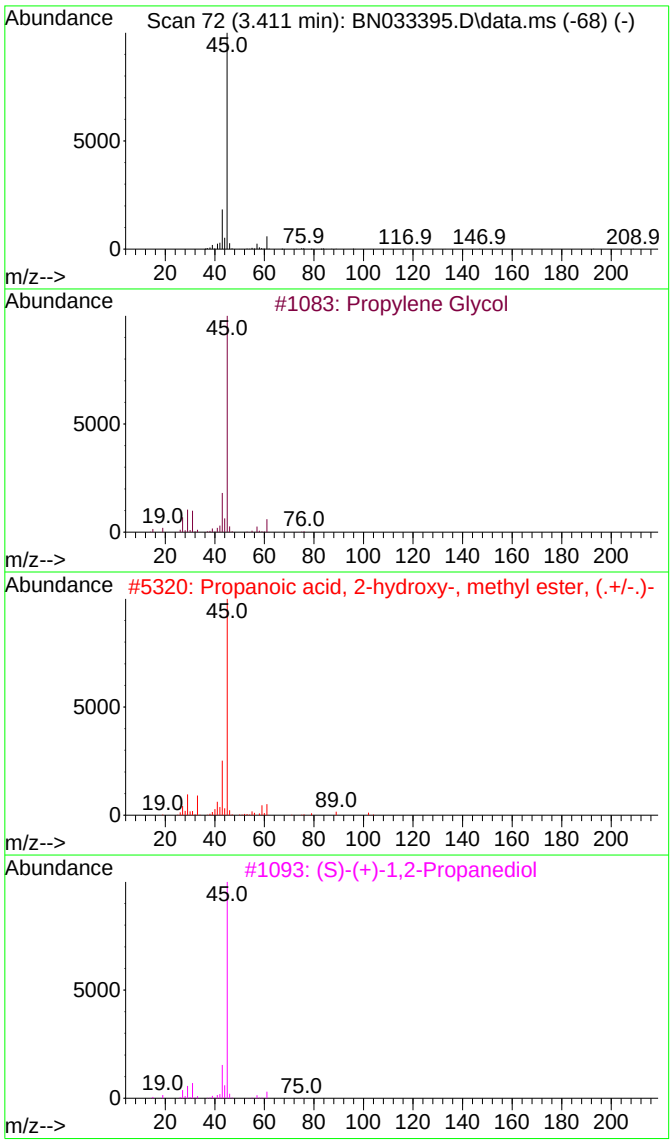
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN081424.MA.M
Quant Title : SVOA CALIBRATION

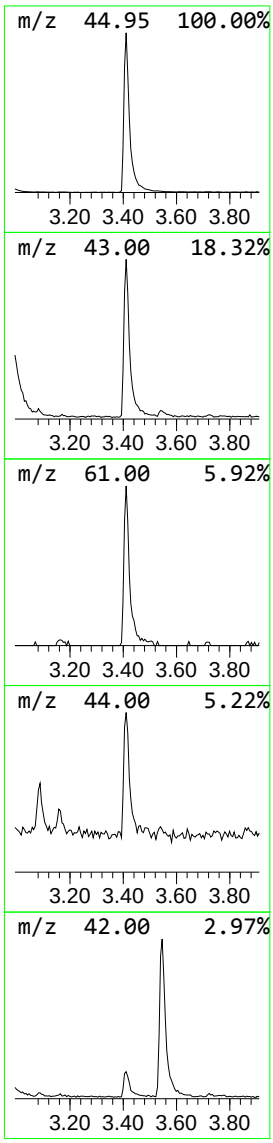
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propylene Glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.411	2.49 ng/ul	305901	1,4-Dichlorobenzene-d4	7.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	90
2	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	32
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081524\
Data File : BN033395.D
Acq On : 15 Aug 2024 11:42
Operator : MA/JU
Sample : P3481-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E0AE2

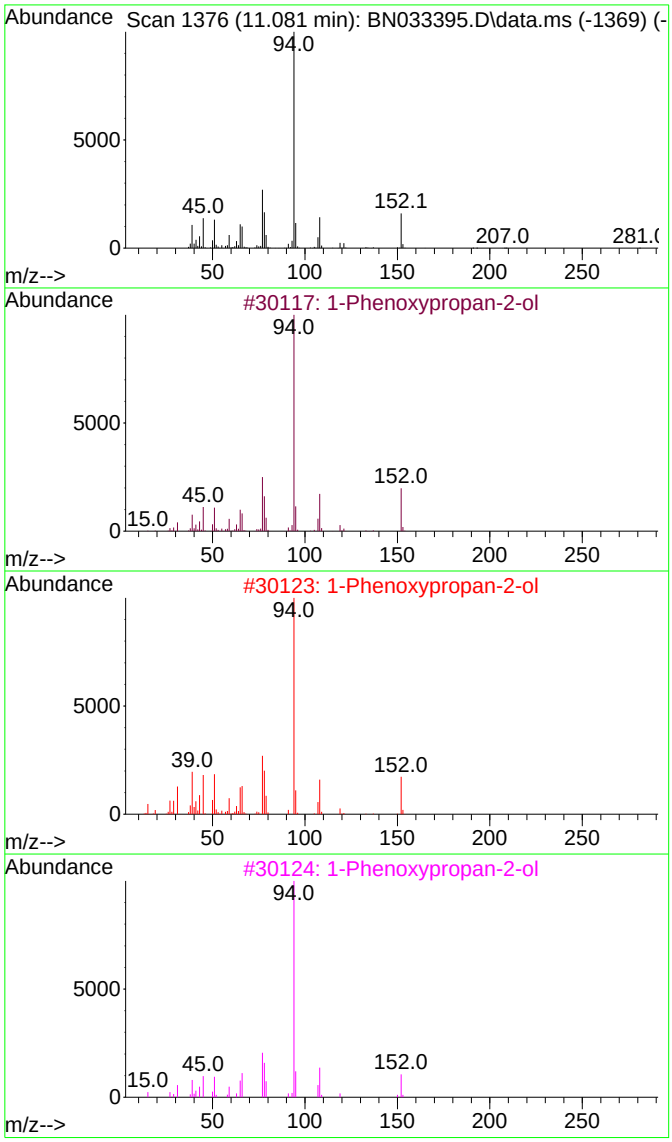
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN081424.MA.M
Quant Title : SVOA CALIBRATION

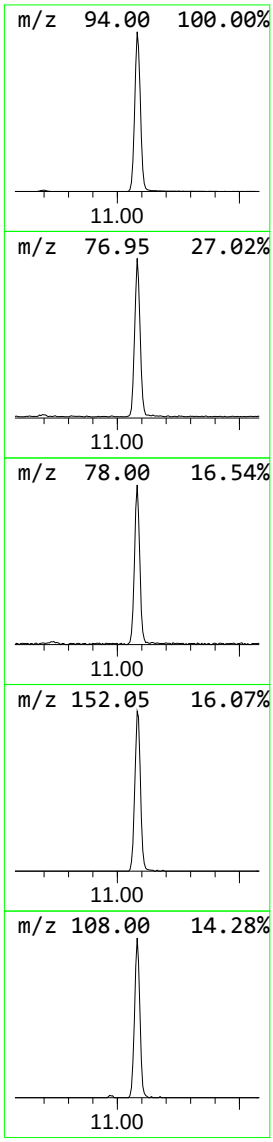
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.081	4.50 ng/ul	871221	Naphthalene-d8	10.334

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	97
2	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
3	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	91
4	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
5	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081524\
Data File : BN033395.D
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Sample : P3481-02
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ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E0AE2

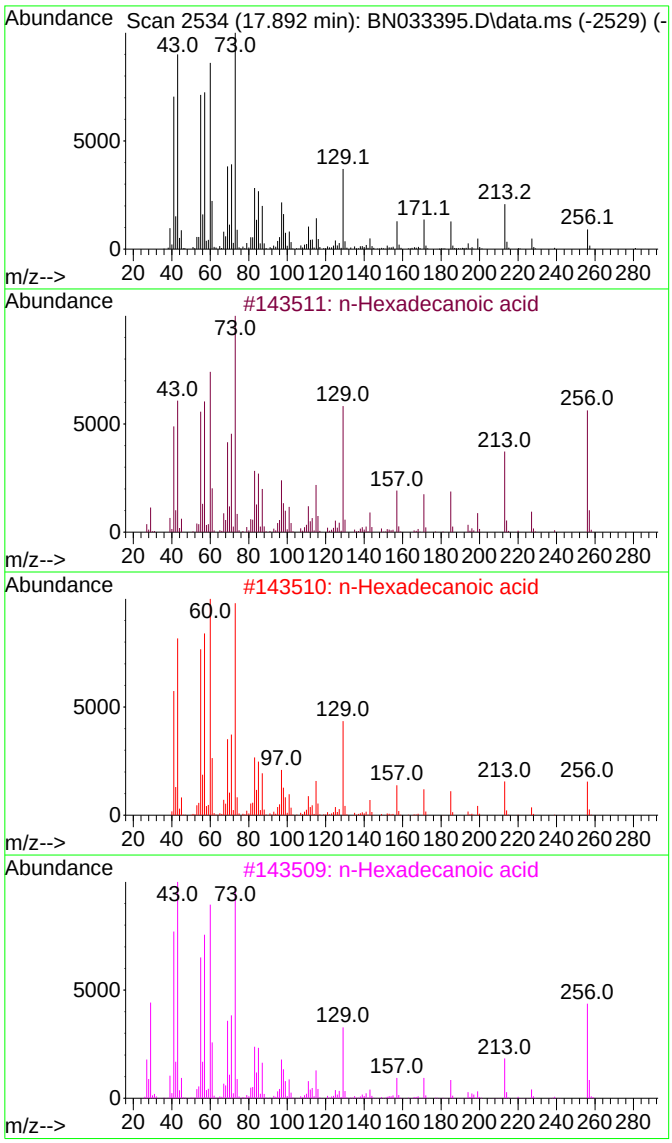
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN081424.MA.M
Quant Title : SVOA CALIBRATION

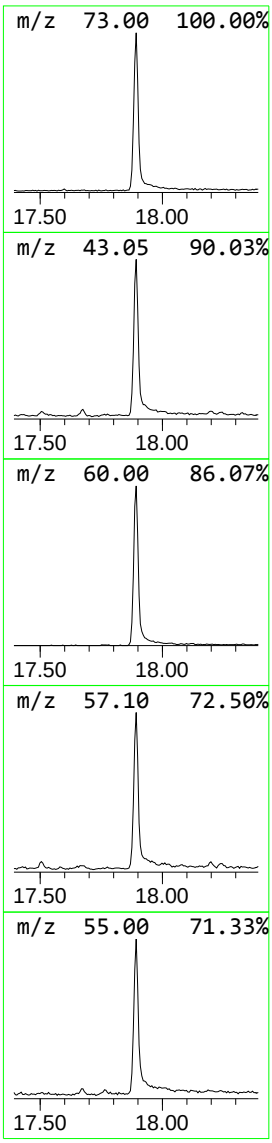
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.892	2.81 ng/ul	877758	Phenanthrene-d10	16.957

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	98
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
5	Tridecanoic acid	214	C13H26O2	000638-53-9	89





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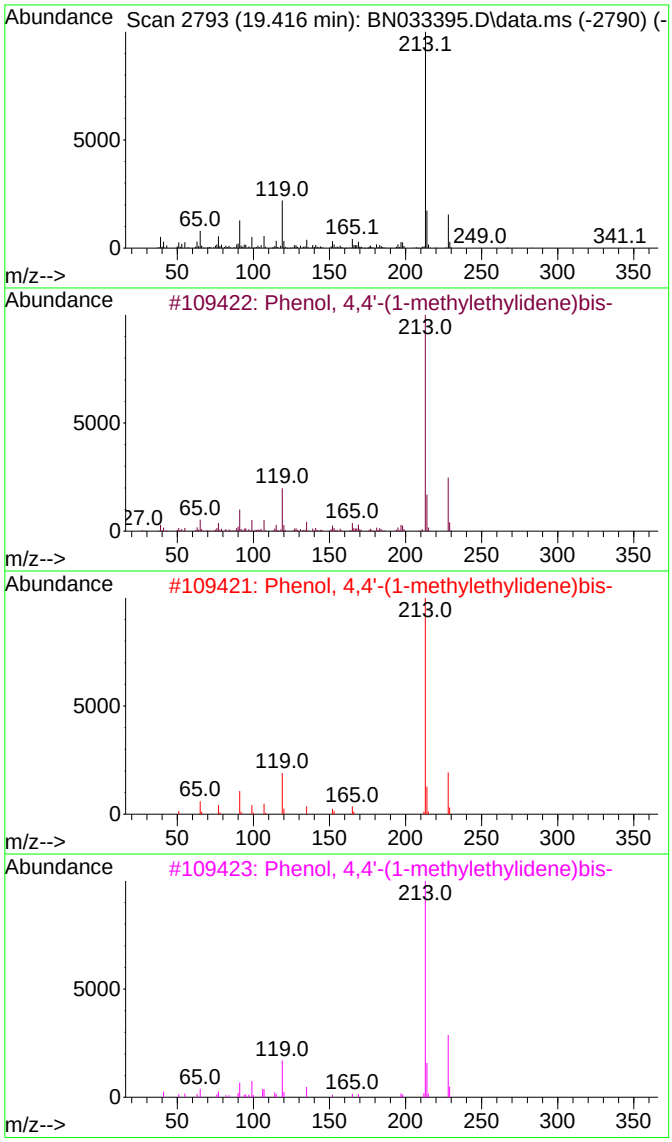
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN081424.MA.M
Quant Title : SVOA CALIBRATION

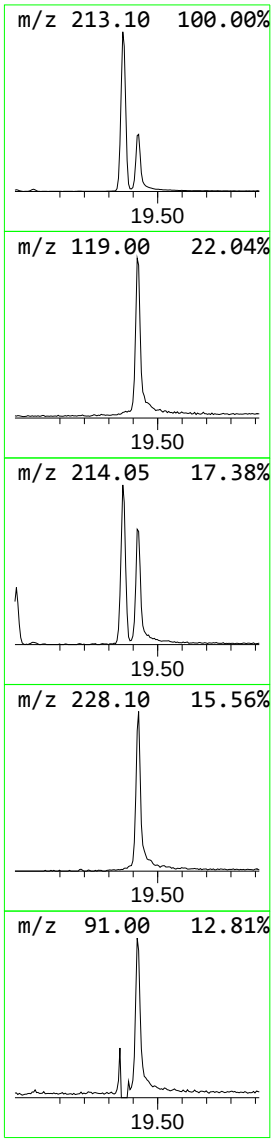
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Phenol, 4,4'-(1-methylethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.416	2.14 ng/ul	721304	Chrysene-d12	21.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	97
2	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96
3	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	87
4	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	83
5	3,4'-Isopropylidenediphenol	228	C15H16O2	046765-25-7	70





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ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E0AE2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN081424.MA.M
Quant Title : SVOA CALIBRATION

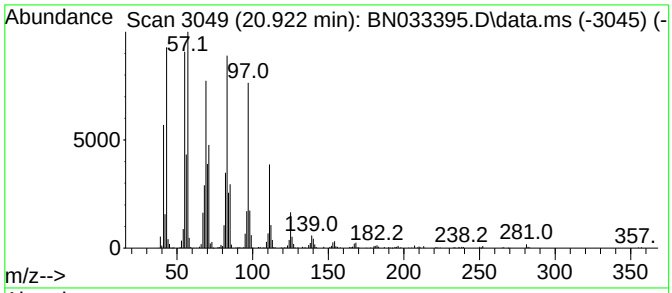
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

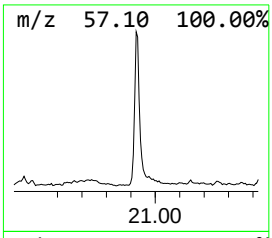
****

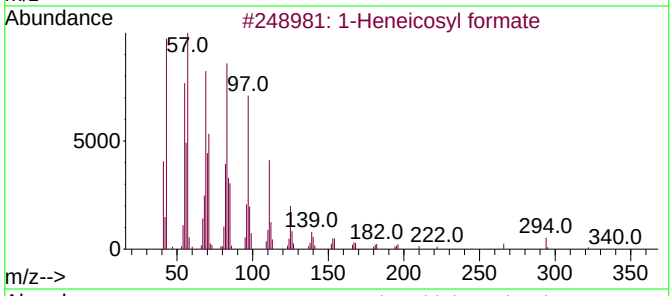
Peak Number 5 1-Heneicosyl formate Concentration Rank 4

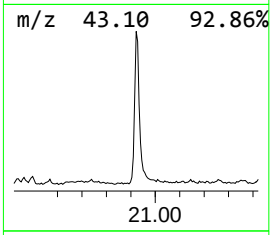
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.922	2.46 ng/ul	827889	Chrysene-d12	21.192

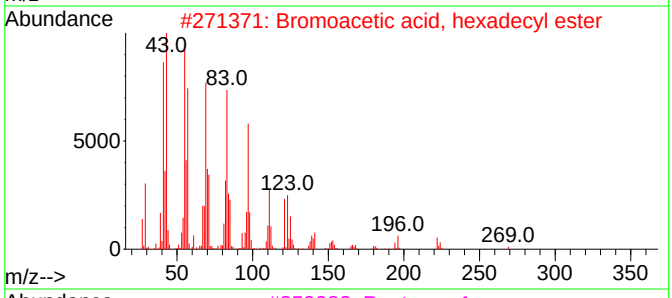
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
3	Pentacos-1-ene	350	C25H50	016980-85-1	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	94

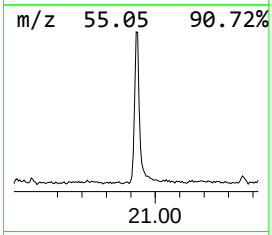


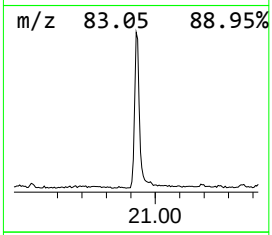


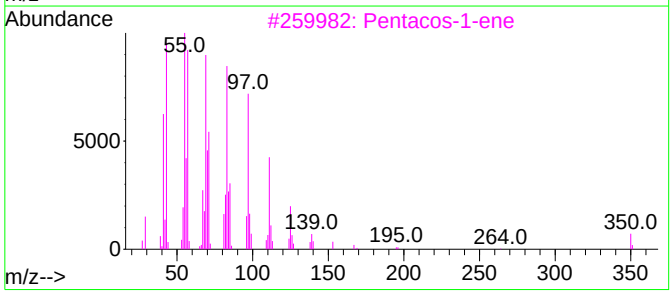


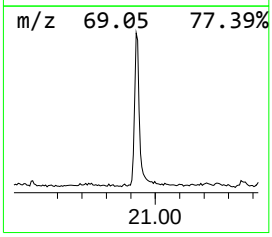












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081524\
Data File : BN033395.D
Acq On : 15 Aug 2024 11:42
Operator : MA/JU
Sample : P3481-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E0AE2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN081424.MA.M
Quant Title : SVOA CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propylene Glycol	3.411	2.5	ng/ul	305901	1	7.569	2457580	20.0
1-Phenoxypropan...	11.081	4.5	ng/ul	871221	2	10.334	3869970	20.0
n-Hexadecanoic ...	17.892	2.8	ng/ul	877758	4	16.957	6250640	20.0
Phenol, 4,4'-(1...	19.416	2.1	ng/ul	721304	5	21.192	6737200	20.0
1-Heneicosyl fo...	20.922	2.5	ng/ul	827889	5	21.192	6737200	20.0