LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092723\
Data File : BP017401.D
Acq On : 27 Sep 2023 17:09
Operator : MA/JU
Sample : 04359-05 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JLAD3

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_P\Methods\SFAM-EPA-BP092023.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP017401.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	12	16	20	rVB	25310	33216	0.63%	0.078%
2	3.322	36	40	47	rVB	265635	304992	5.77%	0.714%
3	3.640	90	94	98	rBV	38918	43984	0.83%	0.103%
4	3.728	106	109	122	rBV2	211986	347355	6.57%	0.813%
5	3.922	138	142	147	rVB	36907	51853	0.98%	0.121%
6	4.016	153	158	166	rBV2	46374	71117	1.35%	0.166%
7	4.187	182	187	192	rVB6	19332	32990	0.62%	0.077%
8	4.293	200	205	210	rVB	57189	77193	1.46%	0.181%
9	4.375	215	219	223	rBV6	10729	17592	0.33%	0.041%
10	4.487	234	238	245	rVV	83023	97994	1.85%	0.229%
11	4.552	245	249	256	rVB	56944	76646	1.45%	0.179%
12	4.940	310	315	323	rBV	128215	168043	3.18%	0.393%
13	5.011	323	327	334	rVB	23323	33674	0.64%	0.079%
14	5.216	358	362	366	rVB6	5441	8400	0.16%	0.020%
15	5.581	422	424	428	rVB4	6727	7552	0.14%	0.018%
16	5.822	462	465	472	rVB5	10302	15539	0.29%	0.036%
17	6.322	545	550	557	rBV4	12231	23044	0.44%	0.054%
18	6.528	581	585	590	rBV9	5718	9720	0.18%	0.023%
19	6.887	643	646	649	rVB5	7139	9314	0.18%	0.022%
20	7.081	673	679	692	rVB2	101815	177760	3.36%	0.416%
21	7.263	704	710	720	rBV	752228	1125329	21.28%	2.634%
22	7.440	734	740	753	rBV	332516	518937	9.81%	1.215%
23	7.540	753	757	762	rVV7	4294	6431	0.12%	0.015%
24	7.922	815	822	833	rBV	507849	833793	15.77%	1.952%
25	8.187	863	867	870	rBV6	5571	8820	0.17%	0.021%
26	8.257	873	879	884	rVB8	5398	12540	0.24%	0.029%
27	8.634	936	943	955	rBV	294737	491531	9.30%	1.151%
28	8.775	961	967	973	rVB3	18251	30980	0.59%	0.073%
29	8.828	973	976	982	rVB8	3908	7148	0.14%	0.017%
30	9.034	1006	1011	1016	rVB7	6437	8876	0.17%	0.021%
31	9.116	1016	1025	1038	rBV	812301	1338818	25.32%	3.134%
32	9.281	1048	1053	1056	rBV	14854	20047	0.38%	0.047%
33	9.346	1063	1064	1070	rVB4	7219	11255	0.21%	0.026%
34	9.481	1084	1087	1092	rBV6	2991	5630	0.11%	0.013%
35	9.834	1140	1147	1158	rBV	291314	473384	8.95%	1.108%
36	10.357	1224	1236	1245	rBV	439862	767454	14.51%	1.796%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092723\
Data File : BP017401.D
Acq On : 27 Sep 2023 17:09
Operator : MA/JU
Sample : 04359-05 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JLAD3

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_P\Methods\SFAM-EPA-BP092023.MA.M
Title : SVOA CALIBRATION

37	10.740	1294	1301	1309	rBV	700521	1168869	22.11%	2.736%
38	10.910	1318	1330	1350	rBV	623322	1100615	20.82%	2.576%
39	11.234	1379	1385	1391	rBV	134446	214709	4.06%	0.503%
40	11.298	1391	1396	1409	rVB	182708	317019	6.00%	0.742%
41	11.498	1424	1430	1431	rBV5	4467	7042	0.13%	0.016%
42	12.104	1527	1533	1537	rBV9	3320	7218	0.14%	0.017%
43	12.263	1554	1560	1567	rVV	121712	199768	3.78%	0.468%
44	12.328	1567	1571	1579	rVB	18532	29023	0.55%	0.068%
45	12.457	1588	1593	1596	rBV3	8046	14252	0.27%	0.033%
46	12.587	1610	1615	1620	rBV9	5532	9803	0.19%	0.023%
47	12.816	1649	1654	1655	rBV4	4504	5859	0.11%	0.014%
48	13.069	1693	1697	1705	rVB4	5062	12524	0.24%	0.029%
49	13.422	1752	1757	1764	rBV	59819	98528	1.86%	0.231%
50	13.539	1774	1777	1782	rVB6	5167	8552	0.16%	0.020%
51	13.622	1788	1791	1797	rVB8	3146	6177	0.12%	0.014%
52	13.998	1848	1855	1871	rBV	1888415	2610492	49.37%	6.111%
53	14.281	1894	1903	1913	rBV	2114502	2962355	56.03%	6.934%
54	14.581	1947	1954	1965	rBV	1044599	1502552	28.42%	3.517%
55	14.834	1992	1997	2001	rBV5	15401	31810	0.60%	0.074%
56	14.981	2020	2022	2026	rVB5	5601	5793	0.11%	0.014%
57	15.081	2036	2039	2046	rVB9	8254	12868	0.24%	0.030%
58	15.398	2089	2093	2096	rVB5	5452	7774	0.15%	0.018%
59	15.581	2116	2124	2140	rBV	2770423	3945196	74.62%	9.235%
60	15.710	2140	2146	2158	rVV	193481	307569	5.82%	0.720%
61	15.816	2161	2164	2169	rVB4	12406	20315	0.38%	0.048%
62	16.163	2218	2223	2224	rBV4	3510	5444	0.10%	0.013%
63	16.298	2242	2246	2250	rVB6	5447	6251	0.12%	0.015%
64	16.363	2253	2257	2262	rBV7	4267	8090	0.15%	0.019%
65	17.022	2364	2369	2375	rBV10	6422	11109	0.21%	0.026%
66	17.139	2382	2389	2394	rBV10	6058	11778	0.22%	0.028%
67	17.351	2419	2425	2436	rBV	1305178	1775916	33.59%	4.157%
68	17.451	2436	2442	2454	rBV	3170492	4452220	84.21%	10.422%
69	17.710	2482	2486	2489	rBV6	3803	5755	0.11%	0.013%
70	18.192	2564	2568	2573	rBV	54600	75282	1.42%	0.176%
71	19.263	2747	2750	2755	rVB2	33232	44071	0.83%	0.103%
72	19.339	2758	2763	2766	rBV	32990	44685	0.85%	0.105%
73	19.433	2776	2779	2785	rBV6	21468	30134	0.57%	0.071%
74	19.698	2818	2824	2832	rBV	4116705	5287323	100.00%	12.377%
75	21.457	3118	3123	3132	rBV	1494874	1934876	36.59%	4.529%
76	23.804	3515	3522	3537	rVB	2680838	5215567	98.64%	12.209%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092723\
Data File : BP017401.D
Acq On : 27 Sep 2023 17:09
Operator : MA/JU
Sample : 04359-05 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JLAD3

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_P\Methods\SFAM-EPA-BP092023.MA.M
Title : SVOA CALIBRATION

77	23.968	3544	3550	3561	rVB	949054	1936523	36.63%	4.533%

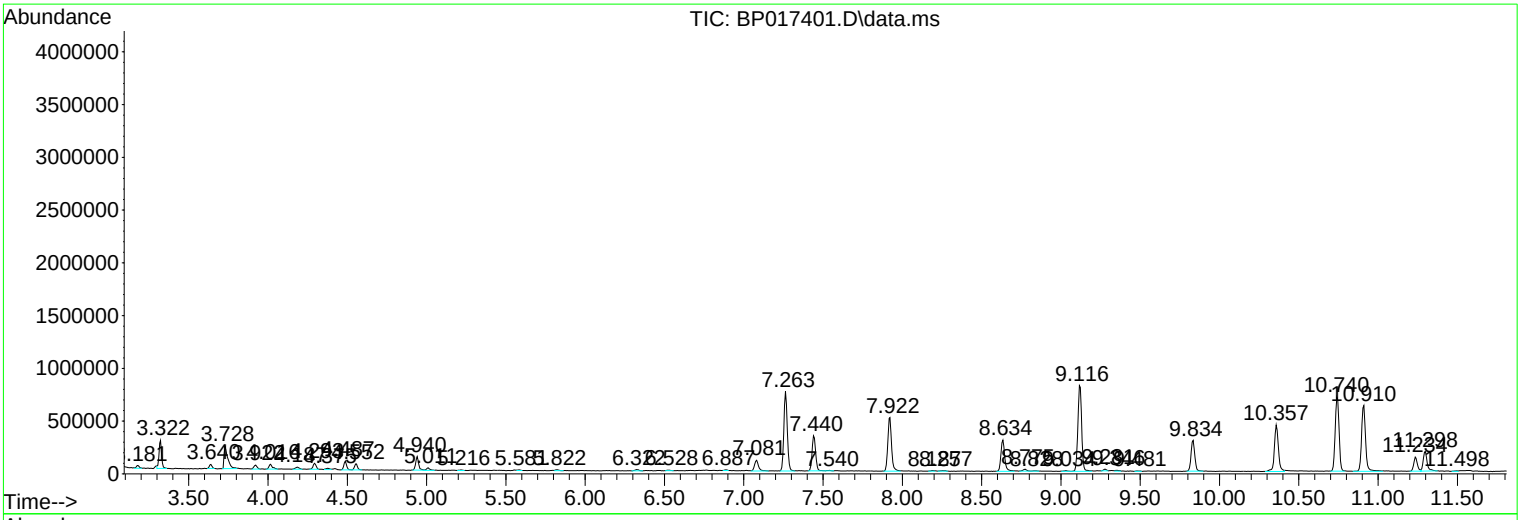
Sum of corrected areas: 42720657

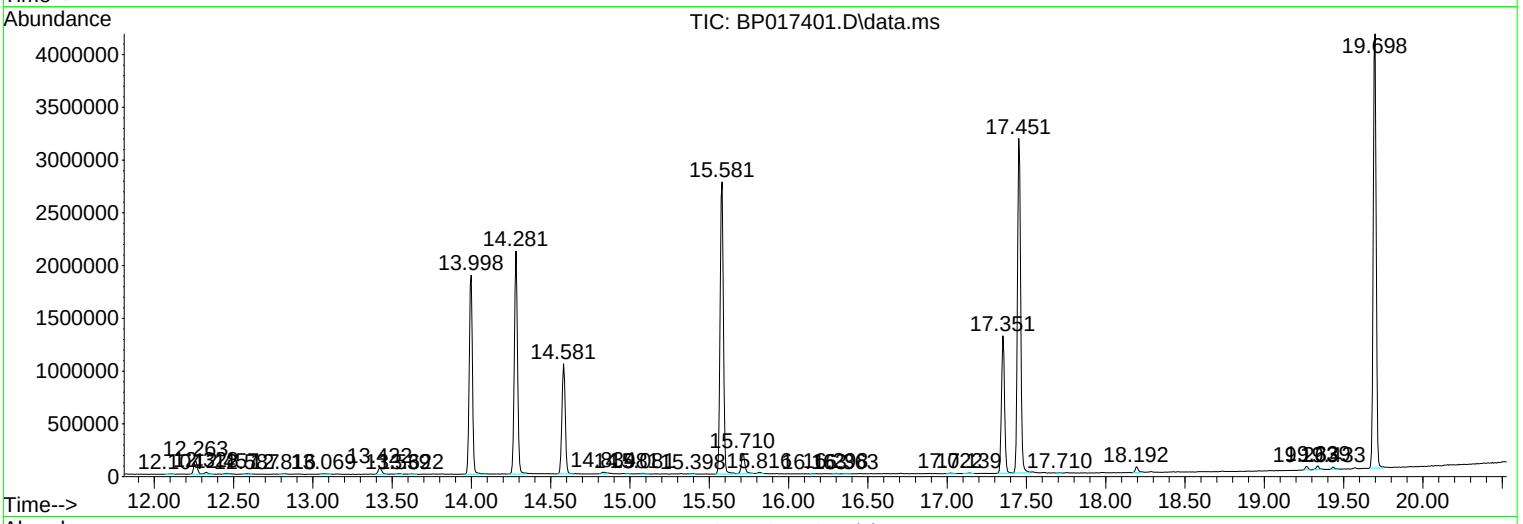
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092723\
Data File : BP017401.D
Acq On : 27 Sep 2023 17:09
Operator : MA/JU
Sample : 04359-05 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

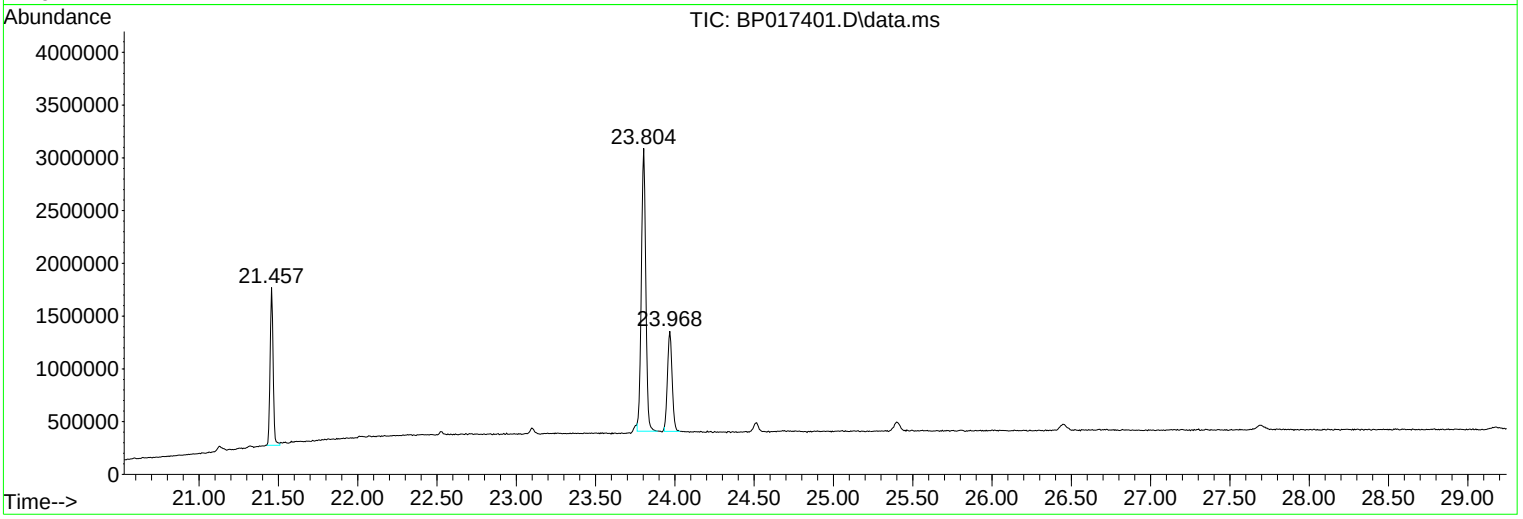
Instrument :
BNA_P
ClientSampleId :
JLAD3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.MA.M
Quant Title : SVOA CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092723\
Data File : BP017401.D
Acq On : 27 Sep 2023 17:09
Operator : MA/JU
Sample : 04359-05 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JLAD3

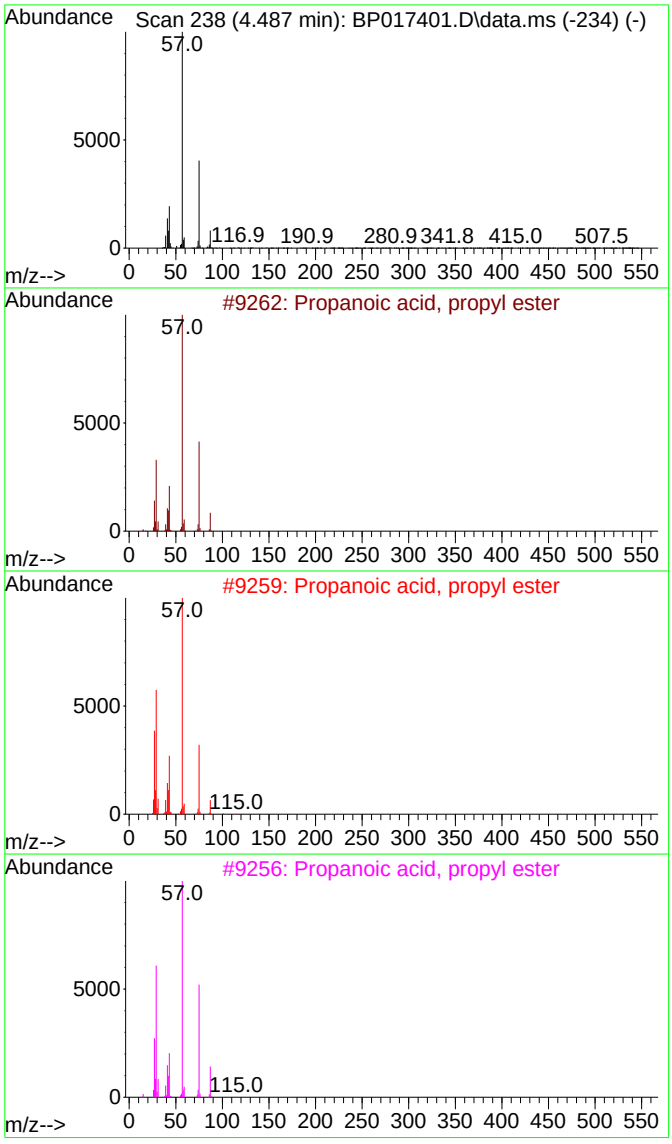
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.MA.M
Quant Title : SVOA CALIBRATION

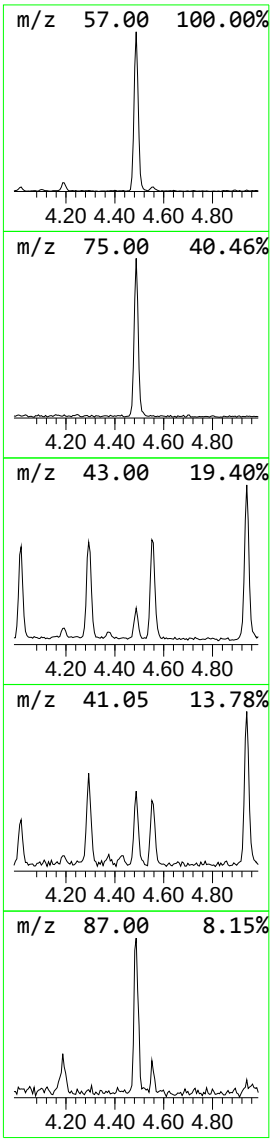
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propanoic acid, propyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.487	2.35 ng/ul	97994	1,4-Dichlorobenzene-d4	7.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
3	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092723\
Data File : BP017401.D
Acq On : 27 Sep 2023 17:09
Operator : MA/JU
Sample : 04359-05 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JLAD3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.MA.M
Quant Title : SVOA CALIBRATION

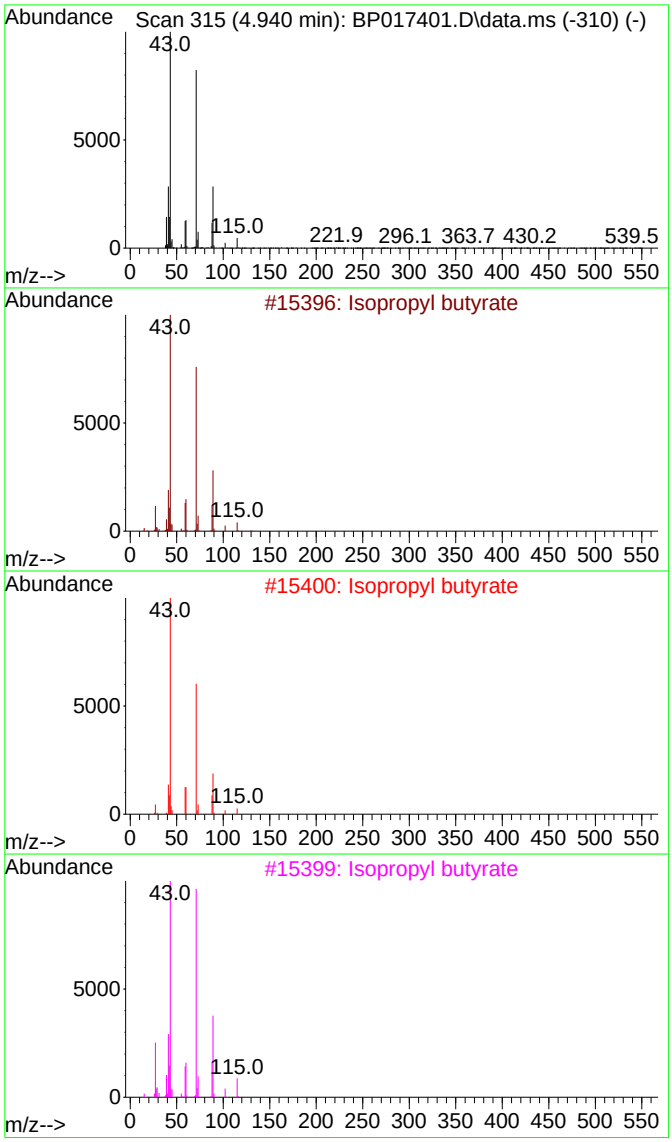
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

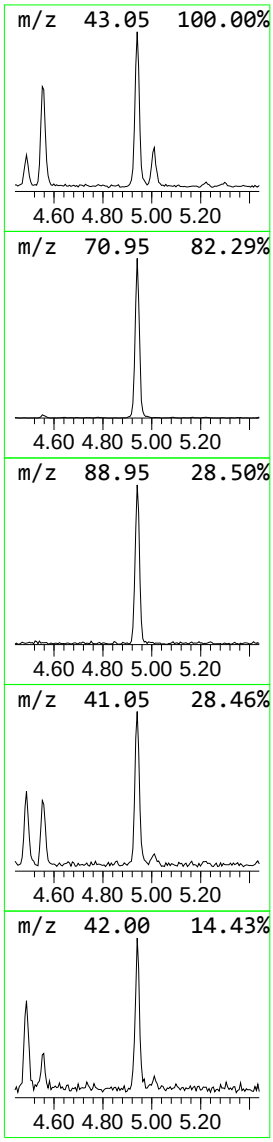
****

Peak Number 2 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.940	4.03 ng/ul	168043	1,4-Dichlorobenzene-d4	7.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	90
2	Isopropyl butyrate	130	C7H14O2	000638-11-9	83
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092723\
Data File : BP017401.D
Acq On : 27 Sep 2023 17:09
Operator : MA/JU
Sample : 04359-05 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JLAD3

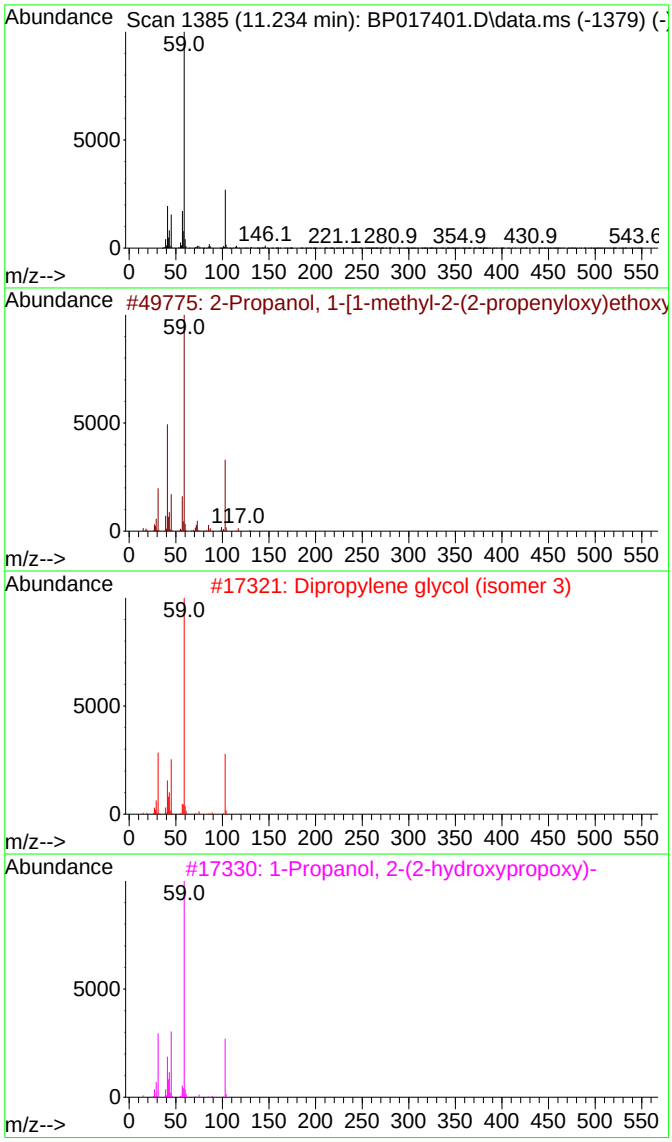
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.MA.M
Quant Title : SVOA CALIBRATION

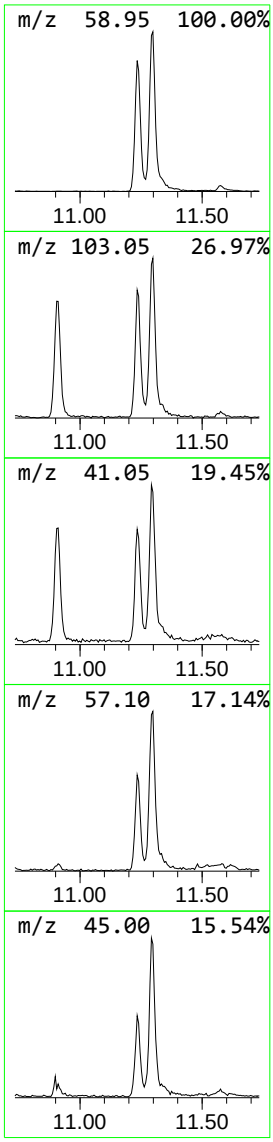
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.234	3.67 ng/ul	214709	Naphthalene-d8	10.740

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64
2	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	64
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64
4	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	64
5	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092723\
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JLAD3

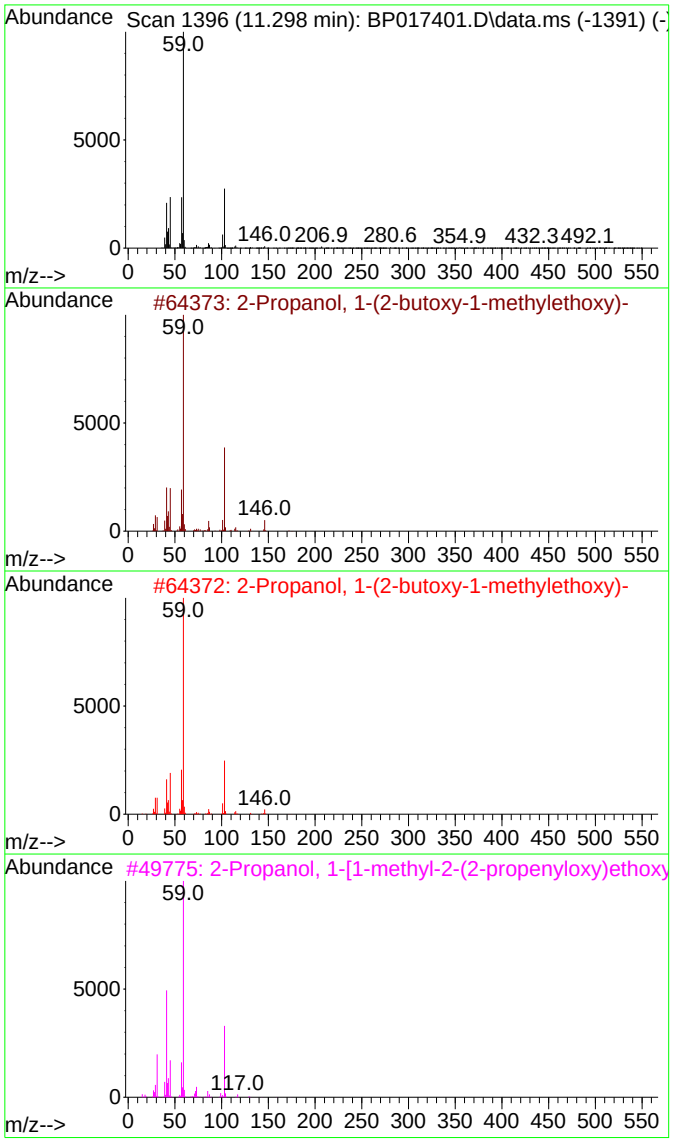
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.MA.M
Quant Title : SVOA CALIBRATION

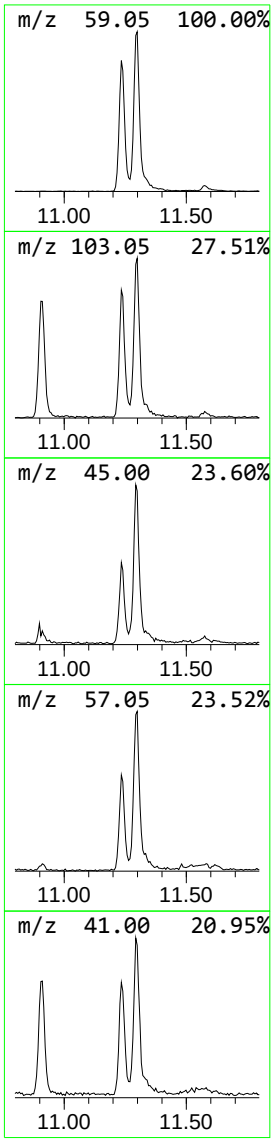
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.298	5.42 ng/ul	317019	Naphthalene-d8	10.740

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	83
2	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	78
3	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	72
4	Methane, diethoxy-	104	C5H12O2	000462-95-3	72
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092723\
Data File : BP017401.D
Acq On : 27 Sep 2023 17:09
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Sample : 04359-05 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JLAD3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.MA.M
Quant Title : SVOA CALIBRATION

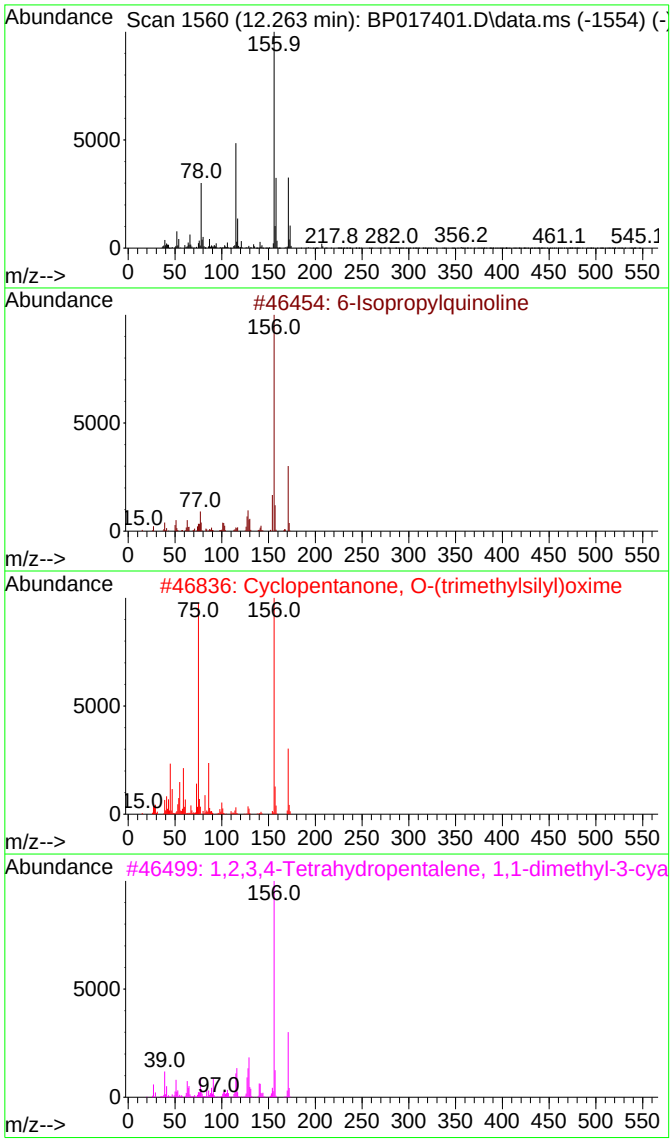
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

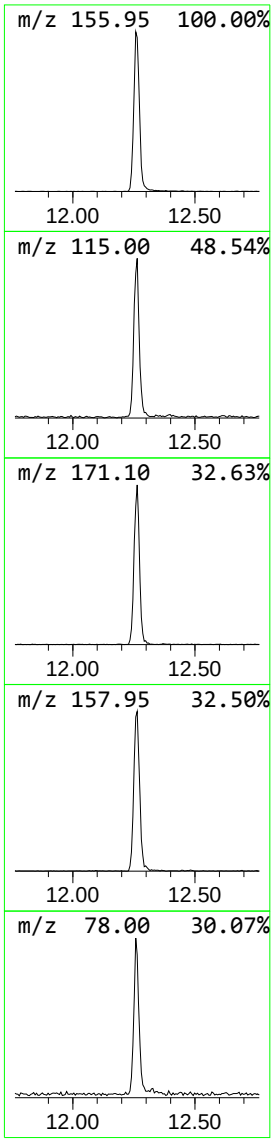
****

Peak Number 5 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.263	3.42 ng/ul	199768	Naphthalene-d8	10.740

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Isopropylquinoline	171	C12H13N	000135-79-5	38
2	Cyclopentanone, O-(trimethylsily...	171	C8H17NOSi	026208-87-7	37
3	1,2,3,4-Tetrahydropentalene, 1,1...	171	C12H13N	1000217-18-6	37
4	2-Chloro-5-hydroxy-2,4,6-cyclohe...	156	C7H5ClO2	007009-16-7	32
5	Chloroxylenol	156	C8H9ClO	000088-04-0	32





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092723\
Data File : BP017401.D
Acq On : 27 Sep 2023 17:09
Operator : MA/JU
Sample : 04359-05 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JLAD3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.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
Propanoic acid,...	4.487	2.4	ng/ul	97994	1	7.922	833793	20.0
Isopropyl butyrate	4.940	4.0	ng/ul	168043	1	7.922	833793	20.0
2-Propanol, 1-[...	11.234	3.7	ng/ul	214709	2	10.740	1168870	20.0
2-Propanol, 1-(...	11.298	5.4	ng/ul	317019	2	10.740	1168870	20.0
unknown-01	12.263	3.4	ng/ul	199768	2	10.740	1168870	20.0