LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102921\
Data File : BP007782.D
Acq On : 29 Oct 2021 13:33
Operator : CG/JU
Sample : M4282-07DL 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BFY76DL

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-BP102521.M
Title : SVOA CALIBRATION

Signal : TIC: BP007782.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.370	12	14	15	rBV2	7668	6735	0.19%	0.021%
2	3.405	16	20	30	rVB	162927	226358	6.25%	0.692%
3	3.676	59	66	75	rBV	83594	153176	4.23%	0.468%
4	3.799	85	87	98	rBV	70400	110843	3.06%	0.339%
5	3.999	116	121	124	rBV	34646	53893	1.49%	0.165%
6	4.111	138	140	146	rVB3	12637	16257	0.45%	0.050%
7	4.805	250	258	268	rVB	105056	216178	5.97%	0.661%
8	4.964	273	285	294	rVV	128639	293266	8.09%	0.897%
9	5.040	294	298	302	rVB6	6018	9302	0.26%	0.028%
10	5.281	337	339	345	rVB7	4199	4898	0.14%	0.015%
11	5.399	351	359	372	rBV	85096	168765	4.66%	0.516%
12	5.734	411	416	417	rBV5	2392	4066	0.11%	0.012%
13	6.334	508	518	525	rBV	92119	192255	5.31%	0.588%
14	6.434	532	535	539	rBV6	5180	6964	0.19%	0.021%
15	6.928	615	619	624	rVV3	12391	20112	0.56%	0.062%
16	7.093	642	647	654	rVB	135687	211940	5.85%	0.648%
17	7.258	669	675	684	rVB	282300	439820	12.14%	1.345%
18	7.458	703	709	717	rBV	339992	551470	15.22%	1.686%
19	7.534	717	722	729	rVB	18145	31134	0.86%	0.095%
20	7.758	758	760	763	rVB3	3593	3918	0.11%	0.012%
21	7.928	781	789	796	rBV	691306	1085231	29.95%	3.319%
22	7.999	796	801	807	rVB	28114	43693	1.21%	0.134%
23	8.469	876	881	882	rBV5	3091	4083	0.11%	0.012%
24	8.640	903	910	917	rBV	313695	517941	14.29%	1.584%
25	8.693	917	919	924	rVB6	9099	13096	0.36%	0.040%
26	9.087	979	986	996	rBV	324249	532830	14.70%	1.629%
27	9.546	1058	1064	1068	rVB3	12239	21118	0.58%	0.065%
28	9.811	1101	1109	1118	rBV	258745	439308	12.12%	1.343%
29	10.358	1194	1202	1217	rBV	433431	736377	20.32%	2.252%
30	10.516	1223	1229	1237	rBV	44335	72953	2.01%	0.223%
31	10.734	1258	1266	1276	rVB	896468	1516196	41.84%	4.637%
32	10.869	1280	1289	1302	rBV	332314	598930	16.53%	1.832%
33	11.140	1333	1335	1342	rVB8	5561	10339	0.29%	0.032%
34	11.928	1466	1469	1472	rBV2	9296	12840	0.35%	0.039%
35	11.999	1472	1481	1484	rVV3	13480	37175	1.03%	0.114%
36	12.040	1486	1488	1496	rVB3	18905	26561	0.73%	0.081%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102921\
Data File : BP007782.D
Acq On : 29 Oct 2021 13:33
Operator : CG/JU
Sample : M4282-07DL 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BFY76DL

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-BP102521.M
Title : SVOA CALIBRATION

37	12.210	1512	1517	1522	rVV5	7536	13865	0.38%	0.042%
38	12.269	1523	1527	1532	rVB3	6217	11071	0.31%	0.034%
39	12.322	1532	1536	1538	rBV4	8310	11498	0.32%	0.035%
40	12.357	1538	1542	1550	rVB2	23612	40078	1.11%	0.123%
41	12.775	1608	1613	1616	rBV7	2463	3647	0.10%	0.011%
42	12.946	1635	1642	1649	rVB7	6256	15643	0.43%	0.048%
43	13.181	1674	1682	1689	rVB9	6080	11936	0.33%	0.037%
44	13.481	1729	1733	1739	rBV8	5360	9546	0.26%	0.029%
45	13.540	1739	1743	1748	rVB8	3918	6456	0.18%	0.020%
46	13.975	1810	1817	1824	rBV	760935	1082472	29.87%	3.310%
47	14.051	1829	1830	1838	rVB8	2892	5200	0.14%	0.016%
48	14.263	1857	1866	1873	rBV	818160	1216479	33.57%	3.720%
49	14.487	1901	1904	1909	rVB3	6316	8300	0.23%	0.025%
50	14.569	1910	1918	1930	rVV	1483617	2122236	58.57%	6.490%
51	14.763	1946	1951	1963	rBV	64760	124691	3.44%	0.381%
52	14.993	1986	1990	1991	rBV4	6327	7638	0.21%	0.023%
53	15.016	1991	1994	2000	rVB4	16046	26033	0.72%	0.080%
54	15.122	2005	2012	2020	rBV2	19652	50736	1.40%	0.155%
55	15.228	2027	2030	2035	rVB7	5671	9033	0.25%	0.028%
56	15.340	2046	2049	2051	rBV4	3739	4587	0.13%	0.014%
57	15.381	2052	2056	2060	rVV2	14019	20329	0.56%	0.062%
58	15.440	2063	2066	2069	rBV5	3114	4335	0.12%	0.013%
59	15.563	2080	2087	2096	rBV	1178803	1679635	46.35%	5.137%
60	15.675	2101	2106	2114	rBV	177802	261824	7.23%	0.801%
61	15.804	2122	2128	2133	rVB3	15711	23314	0.64%	0.071%
62	16.016	2161	2164	2167	rVB4	4146	5665	0.16%	0.017%
63	16.134	2177	2184	2189	rBV9	5659	14403	0.40%	0.044%
64	16.363	2217	2223	2225	rBV7	4066	7721	0.21%	0.024%
65	16.628	2266	2268	2270	rBV3	3556	3947	0.11%	0.012%
66	16.816	2294	2300	2301	rBV6	3975	5497	0.15%	0.017%
67	16.981	2323	2328	2329	rBV4	8799	12539	0.35%	0.038%
68	17.087	2341	2346	2348	rBV4	9257	16800	0.46%	0.051%
69	17.322	2380	2386	2397	rBV	1845589	2693435	74.33%	8.237%
70	17.422	2397	2403	2415	rVV2	1436738	2037835	56.24%	6.232%
71	18.004	2499	2502	2507	rVB7	13696	16388	0.45%	0.050%
72	18.216	2534	2538	2544	rBV2	54790	83820	2.31%	0.256%
73	18.516	2587	2589	2596	rVB8	7192	11551	0.32%	0.035%
74	19.239	2709	2712	2718	rVB6	22766	26399	0.73%	0.081%
75	19.304	2720	2723	2727	rVV2	20743	27942	0.77%	0.085%
76	19.598	2771	2773	2777	rVB5	20726	18961	0.52%	0.058%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102921\
Data File : BP007782.D
Acq On : 29 Oct 2021 13:33
Operator : CG/JU
Sample : M4282-07DL 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BFY76DL

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-BP102521.M
Title : SVOA CALIBRATION

77	19.657	2778	2783	2791	rBV	1909929	2634340	72.70%	8.056%
78	21.133	3031	3034	3037	rBV4	73087	87342	2.41%	0.267%
79	21.416	3077	3082	3088	rBV	2631110	3413206	94.19%	10.438%
80	23.704	3464	3471	3479	rVB2	1384737	2797154	77.19%	8.554%
81	23.863	3491	3498	3511	rVB2	1762501	3623609	100.00%	11.082%

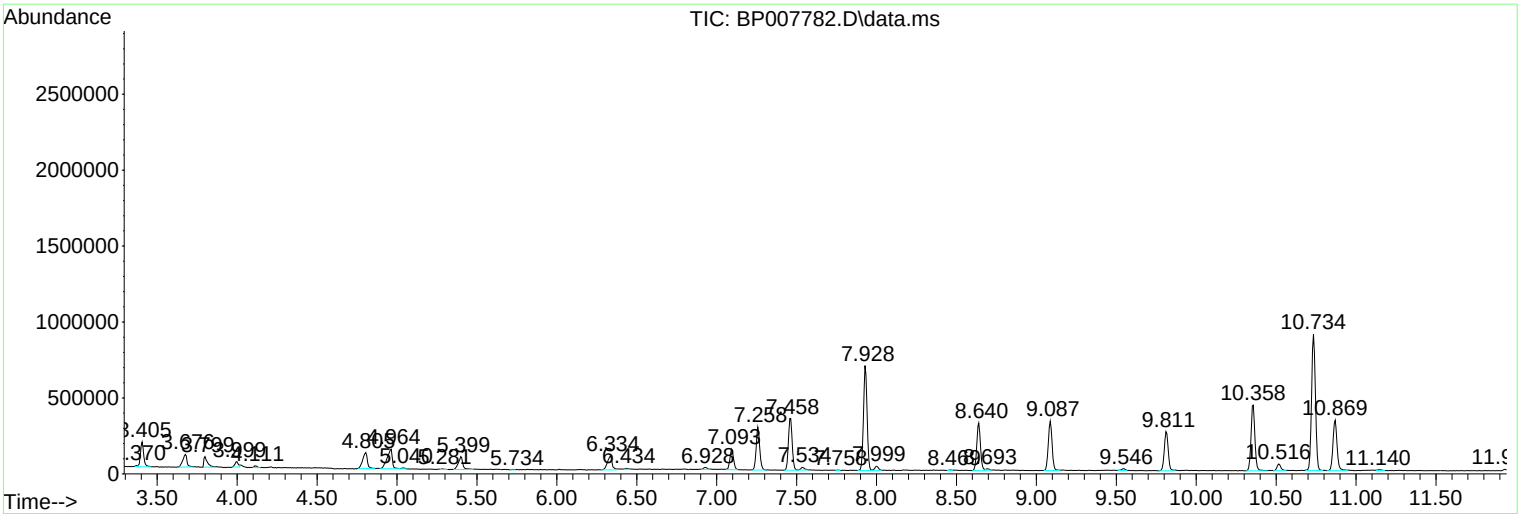
Sum of corrected areas: 32699157

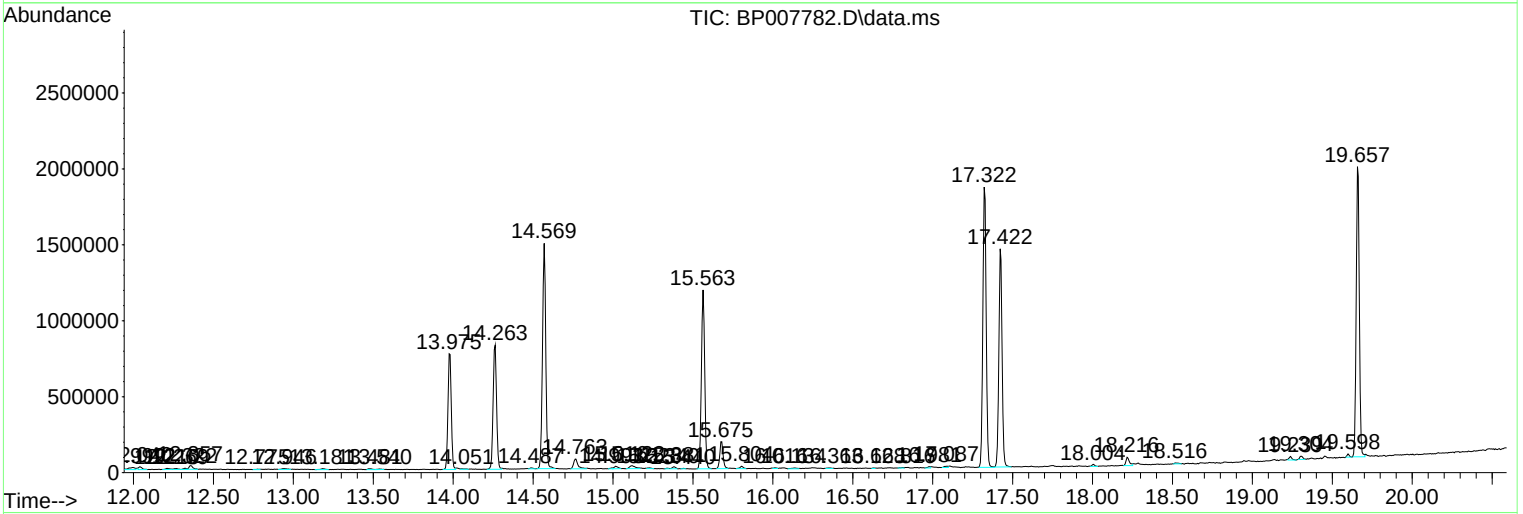
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102921\
Data File : BP007782.D
Acq On : 29 Oct 2021 13:33
Operator : CG/JU
Sample : M4282-07DL 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

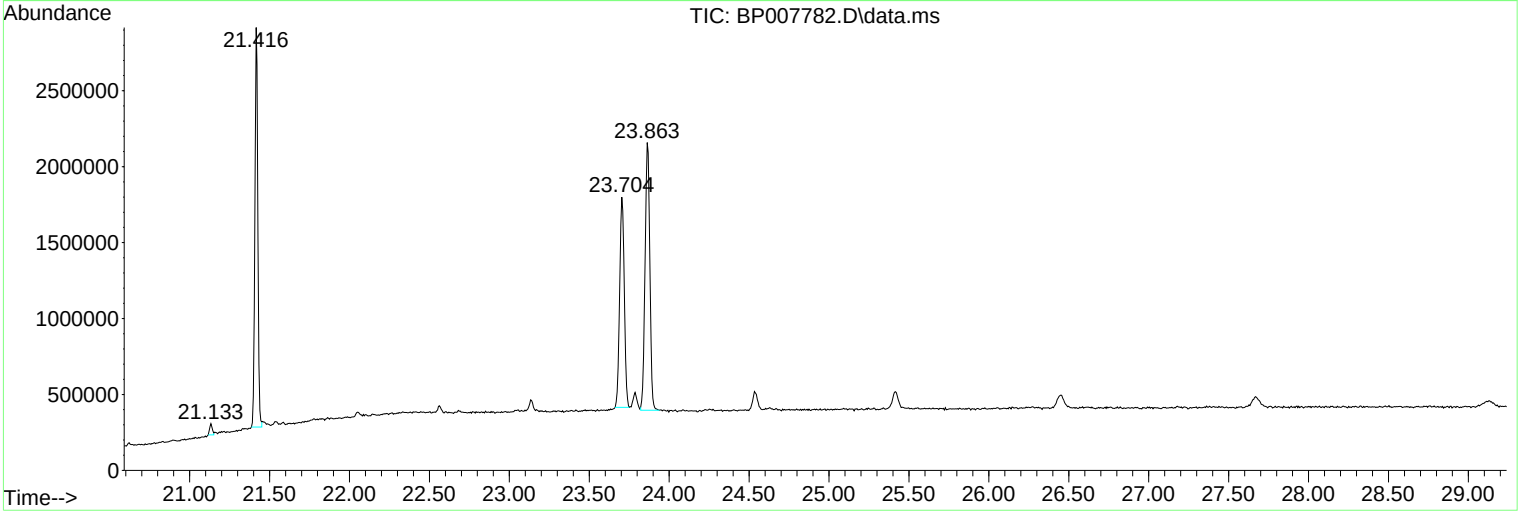
Instrument :
BNA_P
ClientSampleId :
BFY76DL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP102521.M
Quant Title : SVOA CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102921\
Data File : BP007782.D
Acq On : 29 Oct 2021 13:33
Operator : CG/JU
Sample : M4282-07DL 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BFY76DL

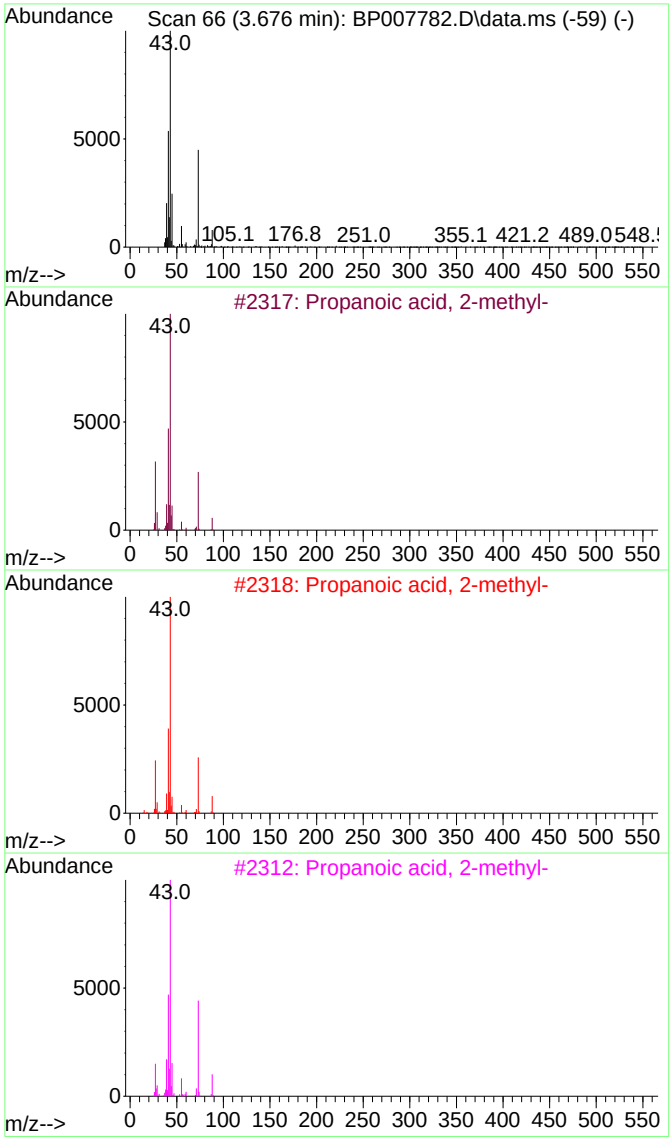
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP102521.M
Quant Title : SVOA CALIBRATION

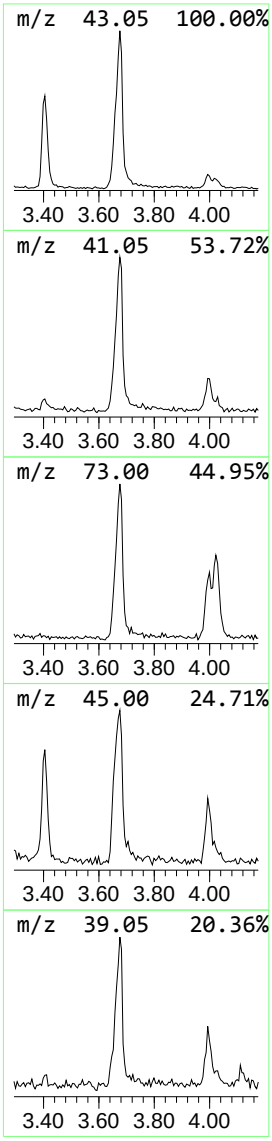
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propanoic acid, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.676	2.82 ng/ul	153176	1,4-Dichlorobenzene-d4	7.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	72
2	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	72
3	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	59
4	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	47
5	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102921\
Data File : BP007782.D
Acq On : 29 Oct 2021 13:33
Operator : CG/JU
Sample : M4282-07DL 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BFY76DL

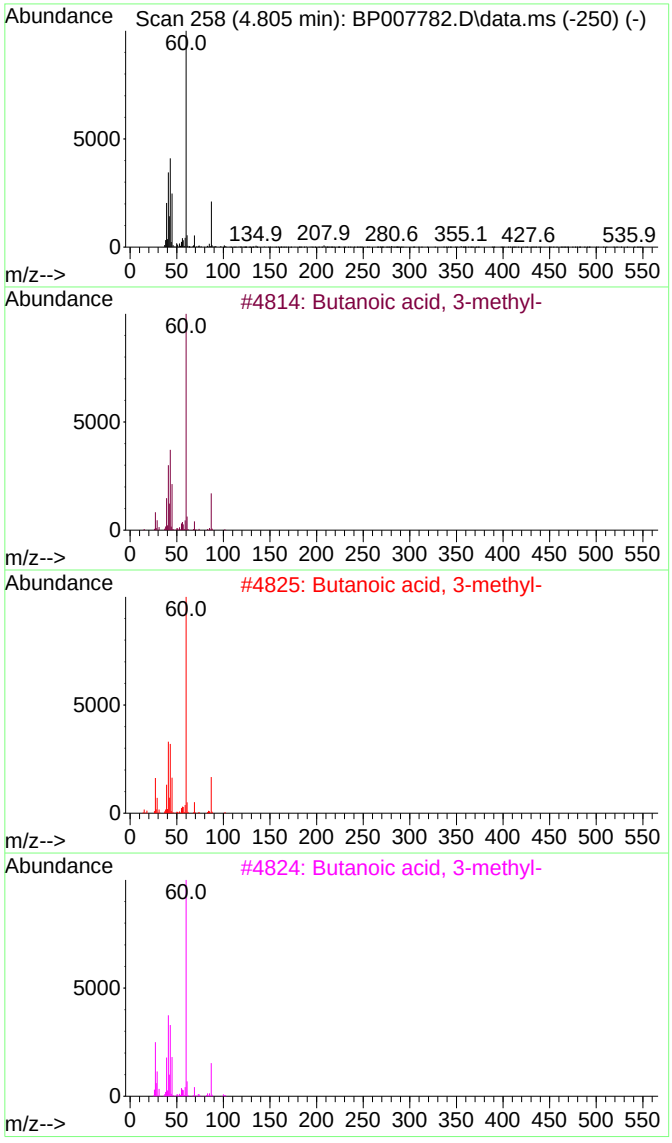
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP102521.M
Quant Title : SVOA CALIBRATION

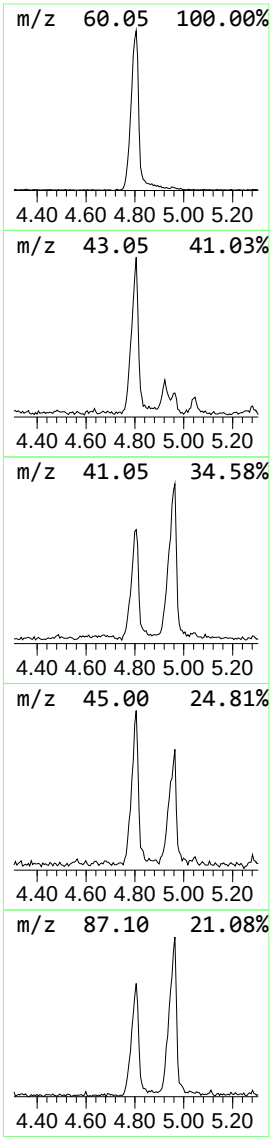
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butanoic acid, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.805	3.98 ng/ul	216178	1,4-Dichlorobenzene-d4	7.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	78
2	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	72
3	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	72
4	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64
5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102921\
Data File : BP007782.D
Acq On : 29 Oct 2021 13:33
Operator : CG/JU
Sample : M4282-07DL 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BFY76DL

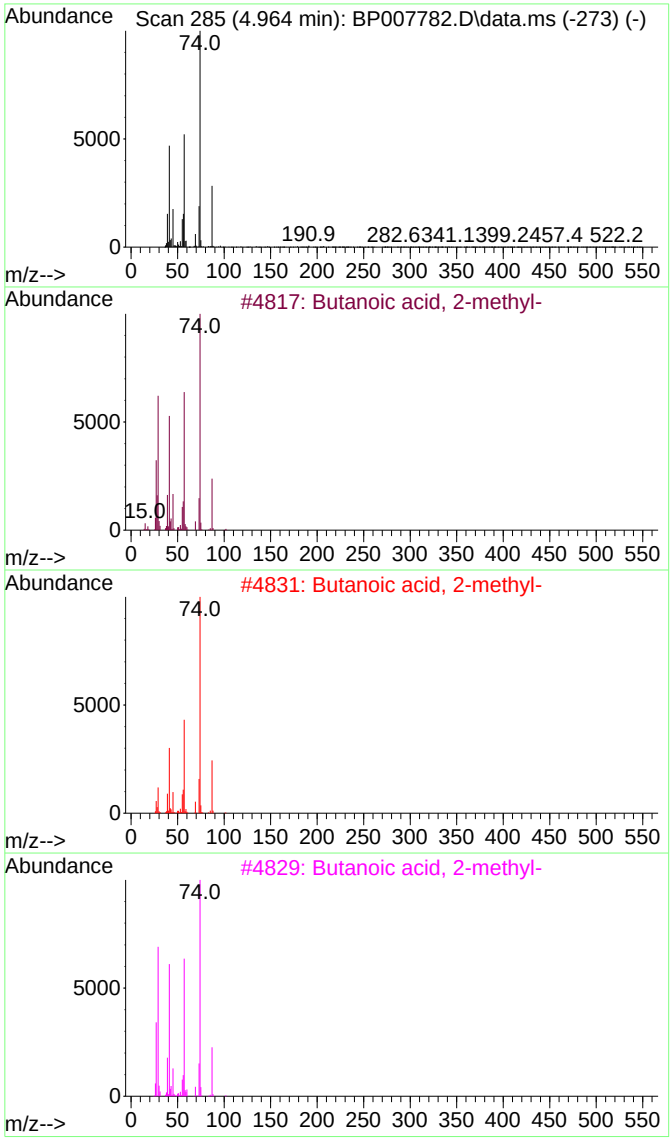
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP102521.M
Quant Title : SVOA CALIBRATION

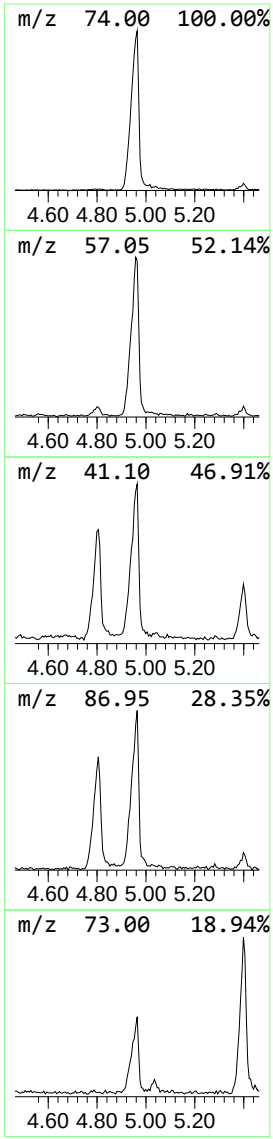
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butanoic acid, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.964	5.40 ng/ul	293266	1,4-Dichlorobenzene-d4	7.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	83
2	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	83
3	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	78
4	2,4-Dimethylpentanoic acid	130	C7H14O2	005868-33-7	56
5	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	56





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102921\
Data File : BP007782.D
Acq On : 29 Oct 2021 13:33
Operator : CG/JU
Sample : M4282-07DL 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BFY76DL

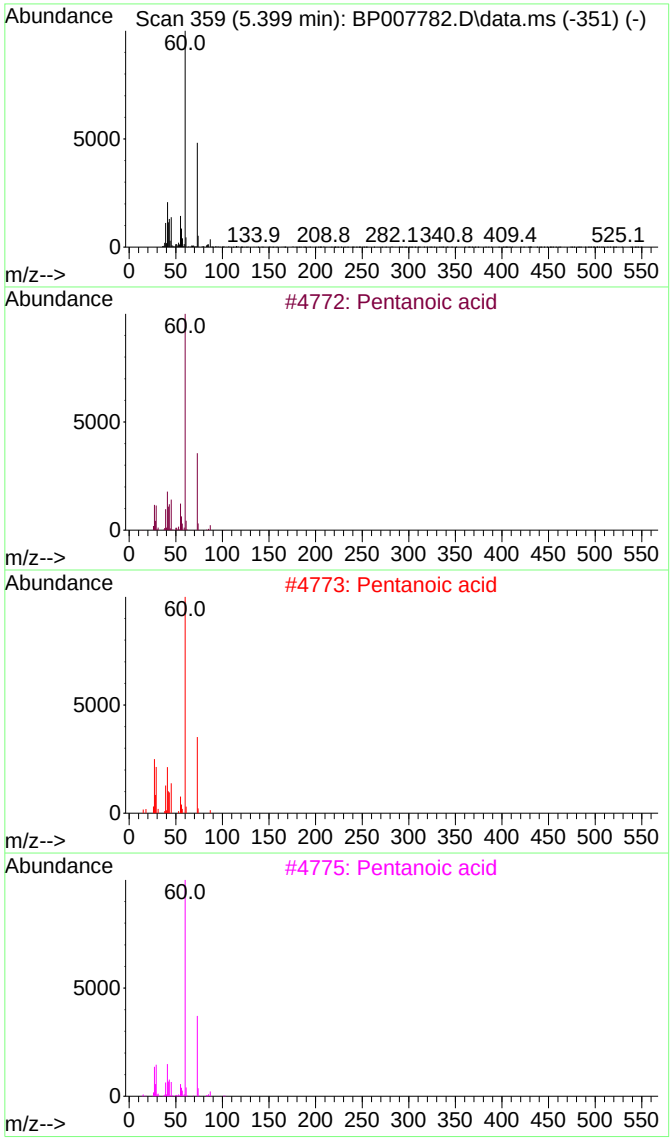
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP102521.M
Quant Title : SVOA CALIBRATION

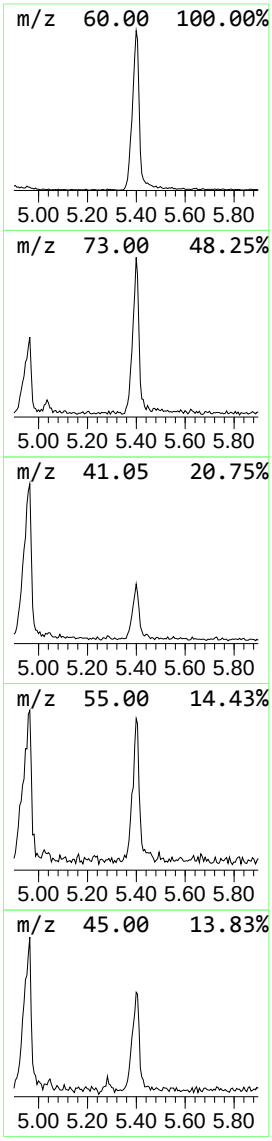
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.399	3.11 ng/ul	168765	1,4-Dichlorobenzene-d4	7.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid	102	C5H10O2	000109-52-4	90
2	Pentanoic acid	102	C5H10O2	000109-52-4	83
3	Pentanoic acid	102	C5H10O2	000109-52-4	83
4	Pentanoic acid	102	C5H10O2	000109-52-4	64
5	Hexanoic acid	116	C6H12O2	000142-62-1	56





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102921\
Data File : BP007782.D
Acq On : 29 Oct 2021 13:33
Operator : CG/JU
Sample : M4282-07DL 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BFY76DL

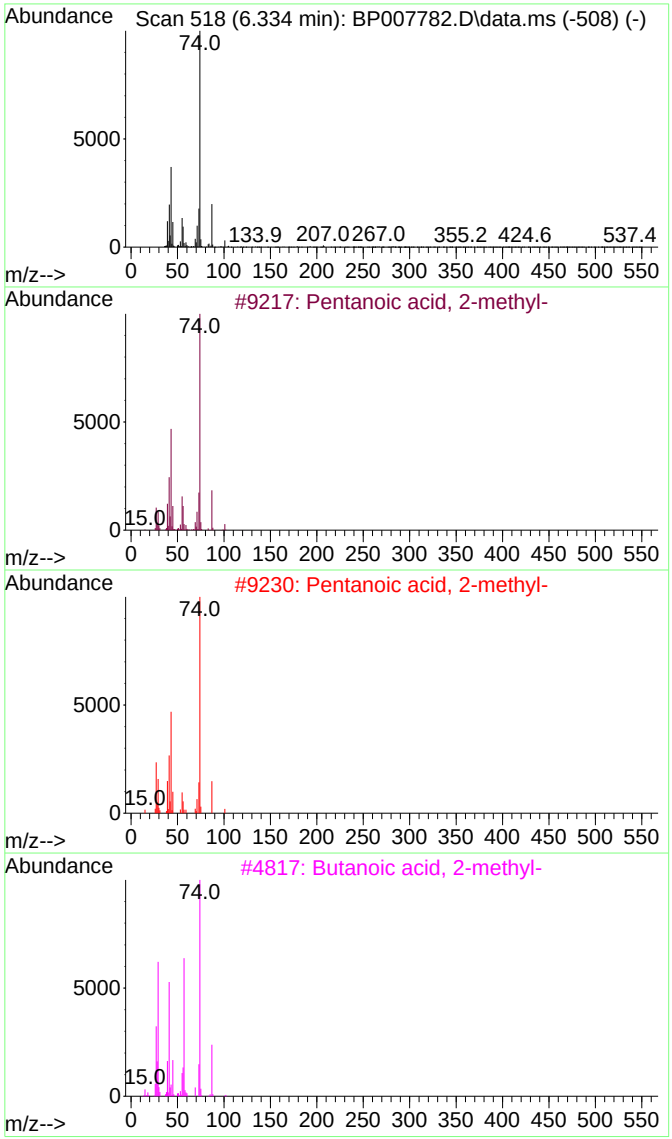
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP102521.M
Quant Title : SVOA CALIBRATION

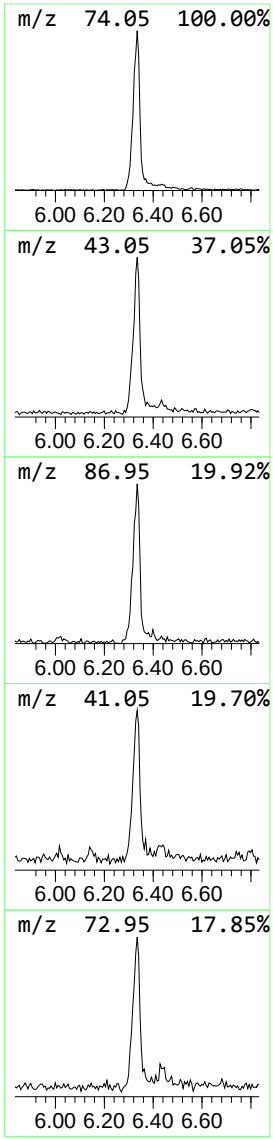
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentanoic acid, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.334	3.54 ng/ul	192255	1,4-Dichlorobenzene-d4	7.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	90
2	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	72
3	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	72
4	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	72
5	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102921\
Data File : BP007782.D
Acq On : 29 Oct 2021 13:33
Operator : CG/JU
Sample : M4282-07DL 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BFY76DL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP102521.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,...	3.676	2.8	ng/ul	153176	1	7.928	1085230	20.0
Butanoic acid, ...	4.805	4.0	ng/ul	216178	1	7.928	1085230	20.0
Butanoic acid, ...	4.964	5.4	ng/ul	293266	1	7.928	1085230	20.0
Pentanoic acid	5.399	3.1	ng/ul	168765	1	7.928	1085230	20.0
Pentanoic acid,...	6.334	3.5	ng/ul	192255	1	7.928	1085230	20.0