LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102121\
Data File : BP007626.D
Acq On : 23 Oct 2021 12:43
Operator : CG/JU
Sample : M4262-13
Misc :
ALS Vial : 86 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BFYA4

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-BP101421.M
Title : SVOA CALIBRATION

Signal : TIC: BP007626.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.376	11	15	17	rBV	47473	55505	0.75%	0.086%
2	3.411	17	21	29	rVB	177454	240296	3.25%	0.373%
3	3.687	59	68	76	rVB	91787	155392	2.10%	0.241%
4	3.793	83	86	101	rBV	203785	351043	4.74%	0.544%
5	4.023	116	125	134	rBV2	112785	221717	2.99%	0.344%
6	4.128	138	143	149	rVB2	13181	22509	0.30%	0.035%
7	4.223	155	159	162	rVB6	13264	16556	0.22%	0.026%
8	4.581	216	220	226	rVB3	7294	13862	0.19%	0.021%
9	4.823	249	261	267	rBV	137609	298301	4.03%	0.462%
10	4.987	276	289	294	rBV	165916	381265	5.15%	0.591%
11	5.423	353	363	369	rBV	119042	253492	3.42%	0.393%
12	6.346	512	520	530	rBV	90346	186537	2.52%	0.289%
13	6.452	534	538	545	rVB8	10237	15313	0.21%	0.024%
14	6.805	592	598	603	rBV9	5551	12151	0.16%	0.019%
15	6.987	615	629	639	rBV	209884	532139	7.19%	0.825%
16	7.111	644	650	658	rVB	257728	398566	5.38%	0.618%
17	7.269	670	677	686	rBV	771017	1221083	16.49%	1.893%
18	7.475	705	712	720	rBV	854522	1343939	18.15%	2.084%
19	7.734	751	756	763	rVB	57065	85605	1.16%	0.133%
20	7.881	774	781	785	rBV	62642	104985	1.42%	0.163%
21	7.940	785	791	799	rVV	719736	1181829	15.96%	1.832%
22	8.017	801	804	811	rVB4	10356	18671	0.25%	0.029%
23	8.187	828	833	839	rVB5	12809	25175	0.34%	0.039%
24	8.381	861	866	868	rBV5	5398	8691	0.12%	0.013%
25	8.516	883	889	900	rVB5	15842	40795	0.55%	0.063%
26	8.652	904	912	918	rBV	713761	1146275	15.48%	1.777%
27	8.711	918	922	929	rVB	54036	88391	1.19%	0.137%
28	9.099	978	988	997	rBV	973519	1622027	21.91%	2.515%
29	9.269	1014	1017	1023	rBV7	4426	7535	0.10%	0.012%
30	9.487	1050	1054	1058	rBV6	4279	7689	0.10%	0.012%
31	9.563	1058	1067	1075	rVB	21771	39132	0.53%	0.061%
32	9.828	1103	1112	1123	rBV	794735	1362295	18.40%	2.112%
33	10.087	1148	1156	1172	rBV	135592	259512	3.51%	0.402%
34	10.369	1196	1204	1212	rBV	1272769	2132456	28.80%	3.306%
35	10.534	1226	1232	1237	rBV3	11089	20298	0.27%	0.031%
36	10.752	1257	1269	1279	rBV	974727	1696180	22.91%	2.630%

LSC Area Percent Report

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Operator : CG/JU
Sample : M4262-13
Misc :
ALS Vial : 86 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BFYA4

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-BP101421.M
Title : SVOA CALIBRATION

37	10.881	1284	1291	1302	rBV	963260	1690043	22.83%	2.620%
38	11.158	1332	1338	1343	rVB9	8056	16771	0.23%	0.026%
39	11.546	1398	1404	1414	rBV9	8686	19609	0.26%	0.030%
40	12.063	1487	1492	1498	rVB2	28649	44046	0.59%	0.068%
41	12.334	1533	1538	1544	rVB2	26837	42100	0.57%	0.065%
42	12.510	1563	1568	1570	rBV6	6311	9635	0.13%	0.015%
43	12.540	1570	1573	1579	rVB4	12562	20290	0.27%	0.031%
44	12.793	1611	1616	1619	rBV7	5317	8578	0.12%	0.013%
45	13.557	1741	1746	1749	rBV7	5935	8383	0.11%	0.013%
46	13.893	1798	1803	1810	rVB2	24519	36661	0.50%	0.057%
47	13.993	1813	1820	1825	rVV	2250577	3178419	42.93%	4.928%
48	14.046	1825	1829	1836	rVV3	21560	41420	0.56%	0.064%
49	14.110	1836	1840	1848	rVB2	12216	20297	0.27%	0.031%
50	14.275	1858	1868	1875	rBV	2528116	3893818	52.59%	6.037%
51	14.334	1876	1878	1886	rVB2	12118	16984	0.23%	0.026%
52	14.469	1895	1901	1903	rBV7	5670	10212	0.14%	0.016%
53	14.534	1909	1912	1914	rBV4	9472	10558	0.14%	0.016%
54	14.581	1914	1920	1925	rVV	1577636	2369073	32.00%	3.673%
55	14.622	1925	1927	1939	rVB	155690	231741	3.13%	0.359%
56	14.775	1947	1953	1963	rVB	247649	377643	5.10%	0.585%
57	14.916	1974	1977	1981	rBV6	4815	9022	0.12%	0.014%
58	15.004	1987	1992	1993	rBV3	26618	35343	0.48%	0.055%
59	15.028	1993	1996	2004	rVV2	37978	71402	0.96%	0.111%
60	15.128	2008	2013	2021	rVB3	18633	40667	0.55%	0.063%
61	15.240	2028	2032	2037	rVB7	10163	15564	0.21%	0.024%
62	15.322	2043	2046	2049	rBV3	7013	10045	0.14%	0.016%
63	15.398	2055	2059	2063	rVB5	7856	10216	0.14%	0.016%
64	15.575	2078	2089	2097	rBV	3498540	4920349	66.46%	7.628%
65	15.687	2102	2108	2117	rBV	780151	1073606	14.50%	1.665%
66	15.816	2125	2130	2138	rVB	42645	66640	0.90%	0.103%
67	16.010	2158	2163	2167	rBV8	10073	21729	0.29%	0.034%
68	16.257	2199	2205	2206	rBV6	8807	14486	0.20%	0.022%
69	17.010	2328	2333	2339	rVB10	7603	13957	0.19%	0.022%
70	17.110	2342	2350	2358	rVV4	11060	34050	0.46%	0.053%
71	17.228	2364	2370	2374	rBV3	26276	48222	0.65%	0.075%
72	17.334	2382	2388	2398	rVB	1977528	2856277	38.58%	4.428%
73	17.434	2398	2405	2418	rBV2	3946237	5734601	77.46%	8.891%
74	17.575	2425	2429	2438	rBV6	12440	24181	0.33%	0.037%
75	17.710	2449	2452	2457	rBV5	7592	11199	0.15%	0.017%
76	17.934	2486	2490	2492	rBV5	6689	8846	0.12%	0.014%

LSC Area Percent Report

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Operator : CG/JU
Sample : M4262-13
Misc :
ALS Vial : 86 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BFYA4

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

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Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP101421.M
Title : SVOA CALIBRATION

77	18.010	2499	2503	2508	rBV7	10522	16026	0.22%	0.025%
78	18.228	2535	2540	2544	rBV2	97232	134278	1.81%	0.208%
79	18.269	2544	2547	2550	rVV5	15940	26843	0.36%	0.042%
80	18.528	2588	2591	2596	rVB6	12860	20379	0.28%	0.032%
81	18.645	2607	2611	2615	rBV2	38350	48400	0.65%	0.075%
82	18.681	2615	2617	2621	rBV5	8363	10686	0.14%	0.017%
83	19.245	2709	2713	2716	rBV2	60433	79270	1.07%	0.123%
84	19.310	2720	2724	2728	rBV	67640	88746	1.20%	0.138%
85	19.457	2746	2749	2757	rBV5	51077	82307	1.11%	0.128%
86	19.669	2779	2785	2791	rBV	5227949	7010621	94.69%	10.869%
87	19.792	2802	2806	2810	rBV	114104	126397	1.71%	0.196%
88	21.422	3078	3083	3088	rBV	2634652	3382752	45.69%	5.245%
89	23.710	3465	3472	3481	rVB2	3690746	7403452	100.00%	11.478%
90	23.869	3492	3499	3509	rVB2	1644346	3436121	46.41%	5.327%

Sum of corrected areas: 64500168

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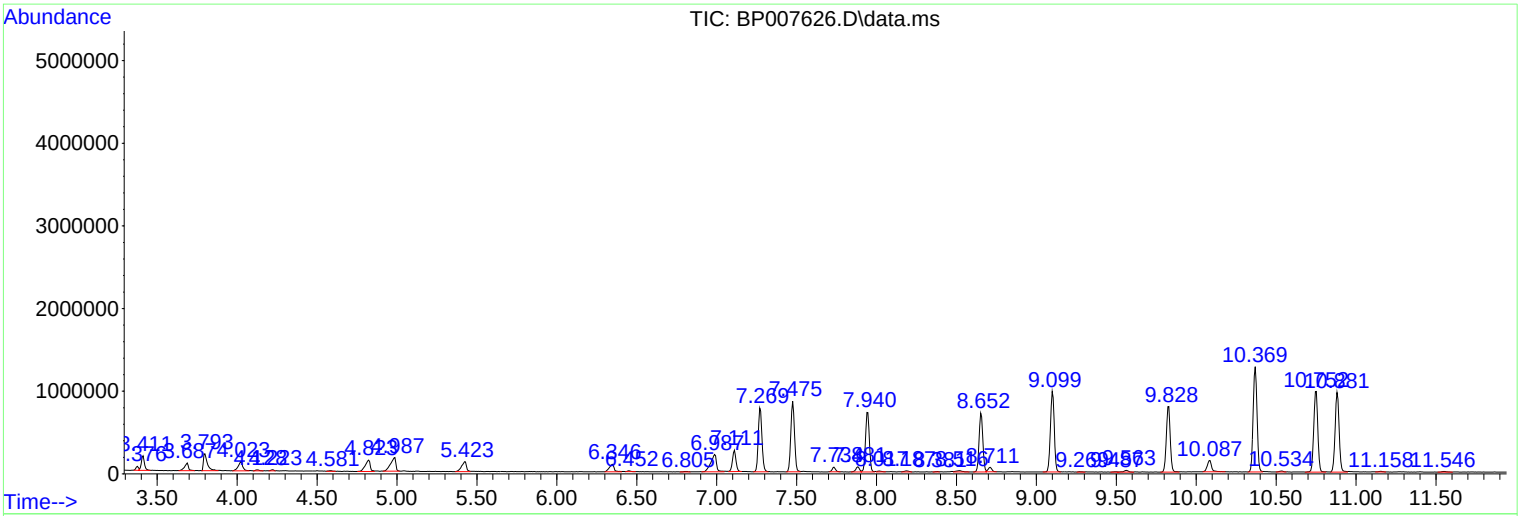
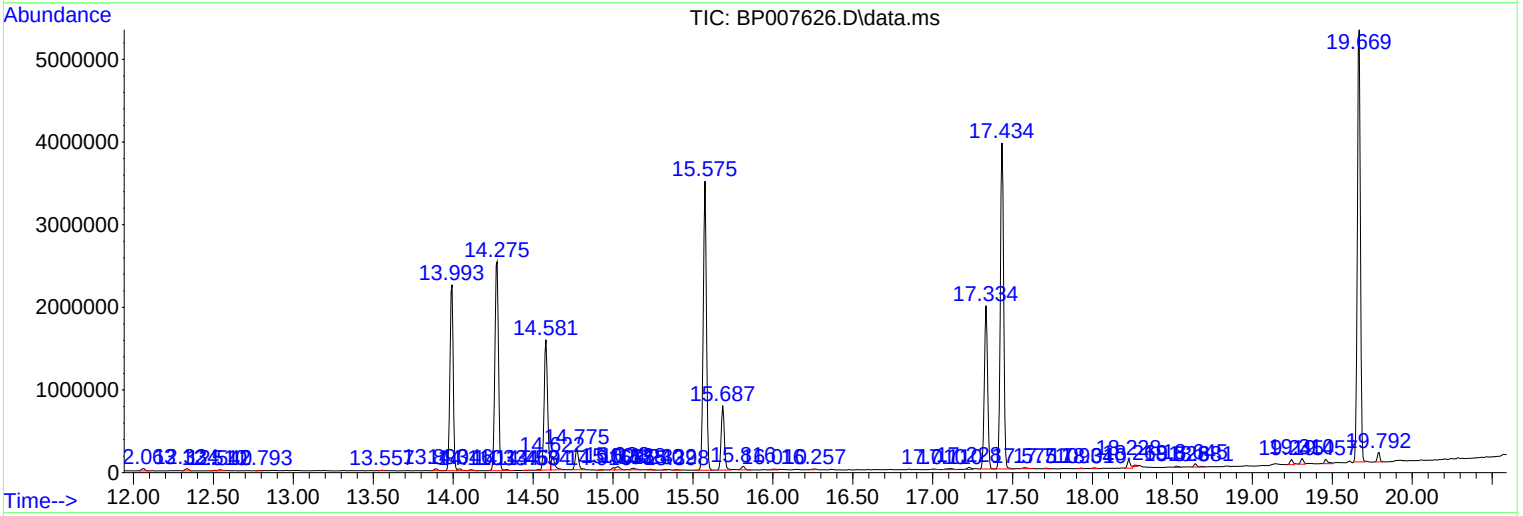
Misc :
ALS Vial : 86 Sample Multiplier: 1

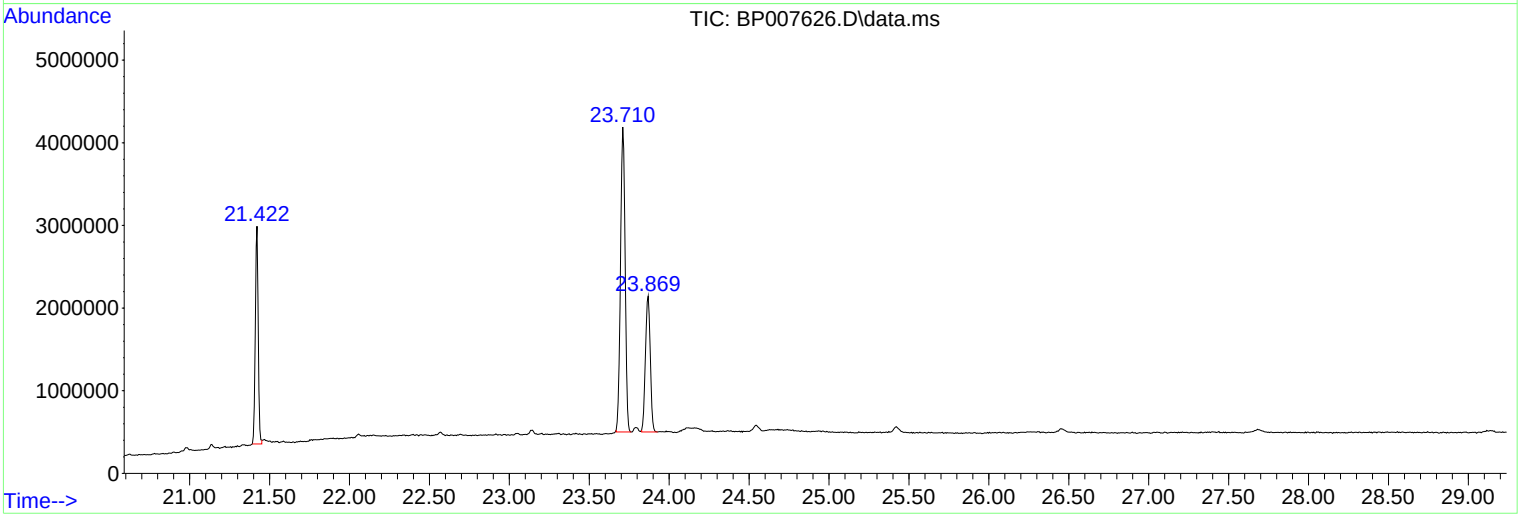
Instrument :
BNA_P
ClientSampleId :
BFYA4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP101421.M
Quant Title : SVOA CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102121\
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Operator : CG/JU
Sample : M4262-13
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ALS Vial : 86 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BFYA4

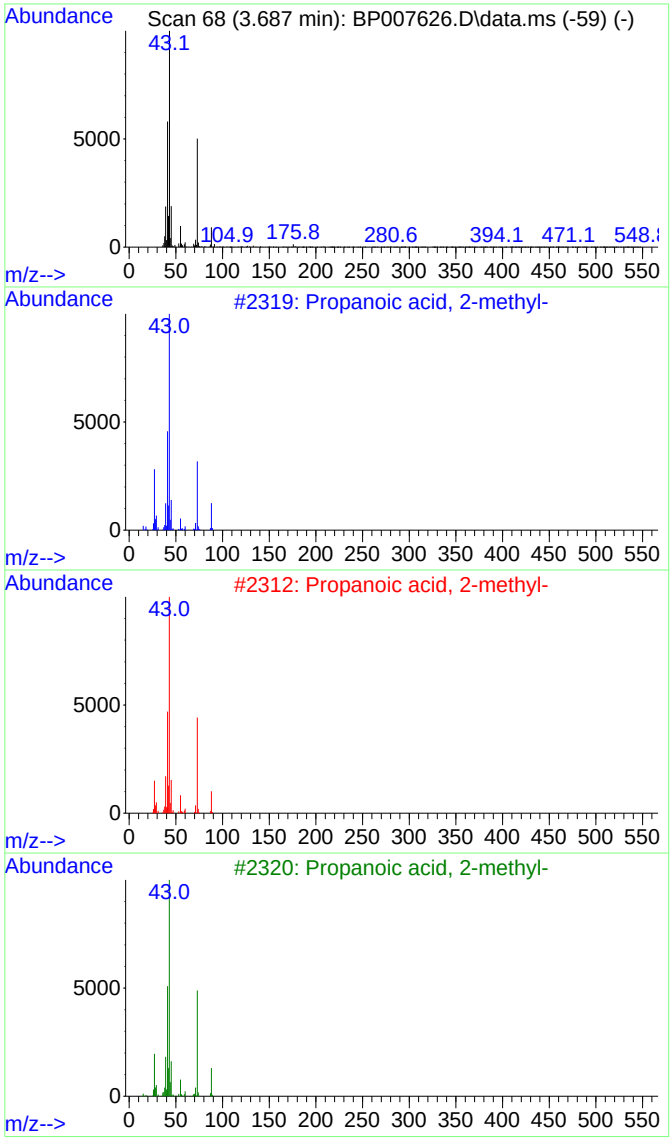
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP101421.M
Quant Title : SVOA CALIBRATION

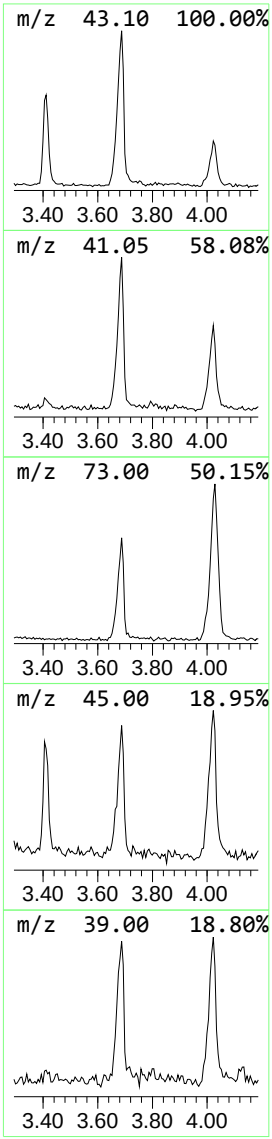
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propanoic acid, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.687	2.63 ng/ul	155392	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	83
2	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	81
3	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	72
4	CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	59
5	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102121\
Data File : BP007626.D
Acq On : 23 Oct 2021 12:43
Operator : CG/JU
Sample : M4262-13
Misc :
ALS Vial : 86 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BFYA4

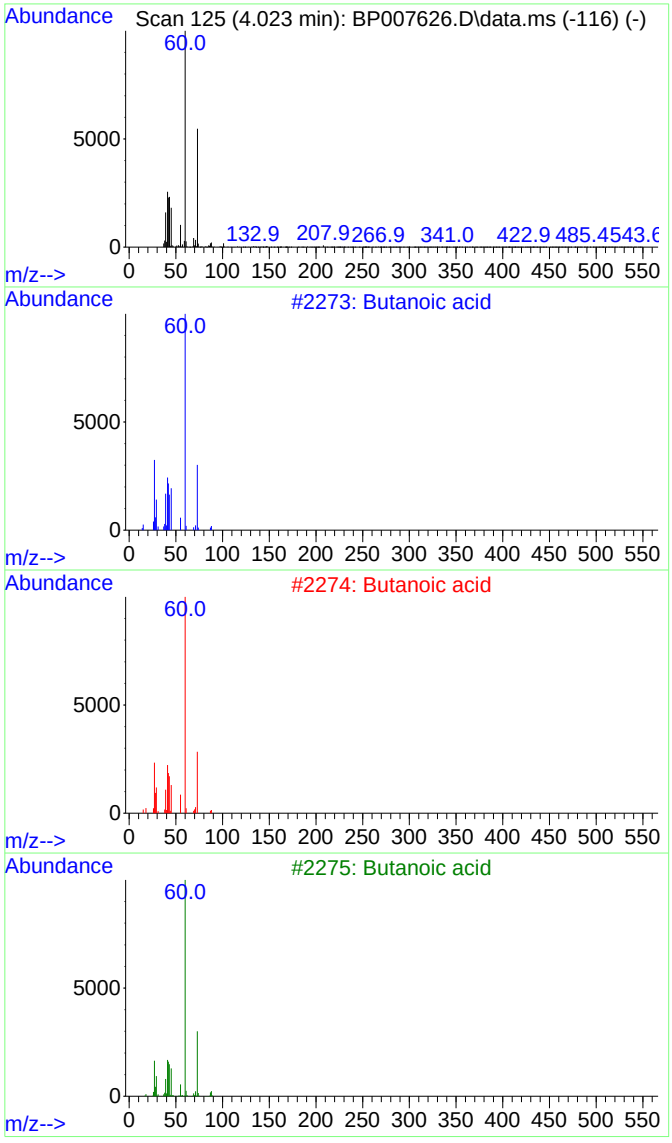
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP101421.M
Quant Title : SVOA CALIBRATION

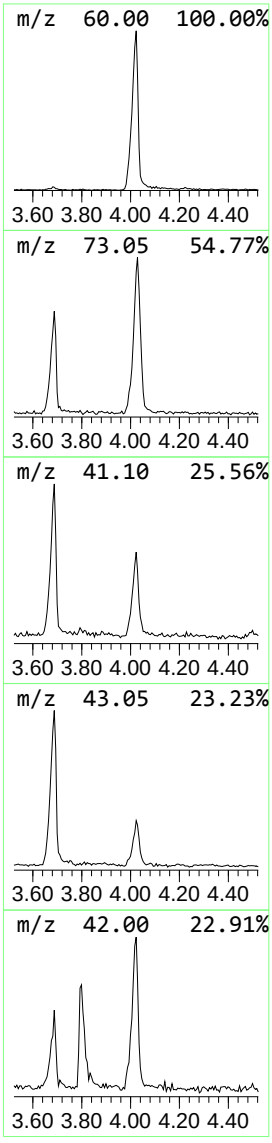
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.023	3.75 ng/ul	221717	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	91
2	Butanoic acid	88	C4H8O2	000107-92-6	90
3	Butanoic acid	88	C4H8O2	000107-92-6	90
4	Butanoic acid	88	C4H8O2	000107-92-6	86
5	Silver butanoate	194	C4H7AgO2	005076-24-4	64





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Instrument :
BNA_P
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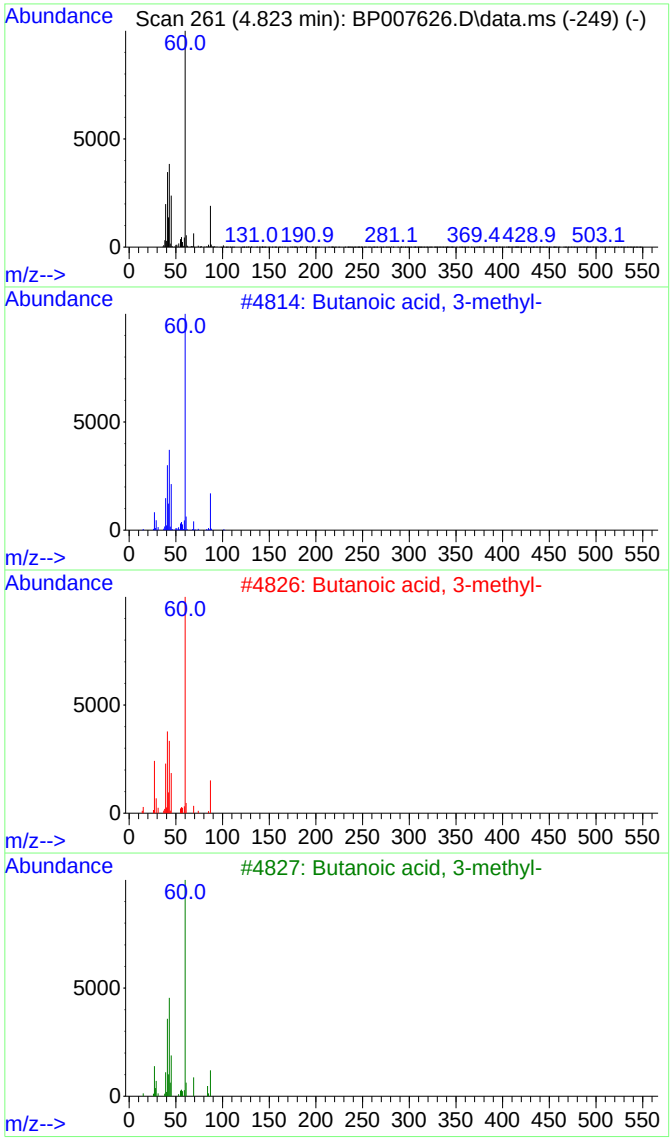
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP101421.M
Quant Title : SVOA CALIBRATION

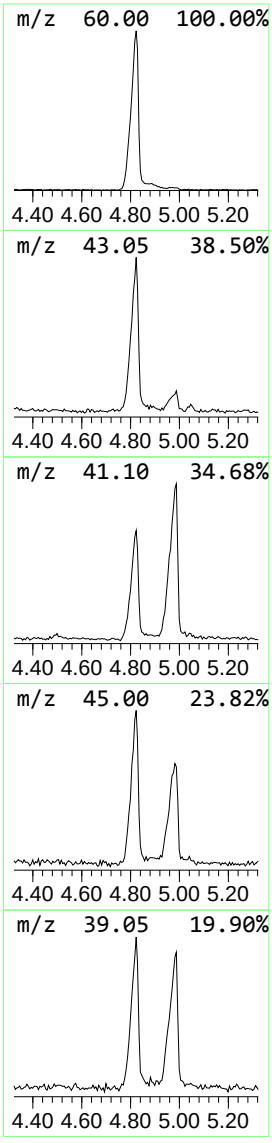
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.823	5.05 ng/ul	298301	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	90
2	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	83
3	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64
4	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64
5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	59





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Sample : M4262-13
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ALS Vial : 86 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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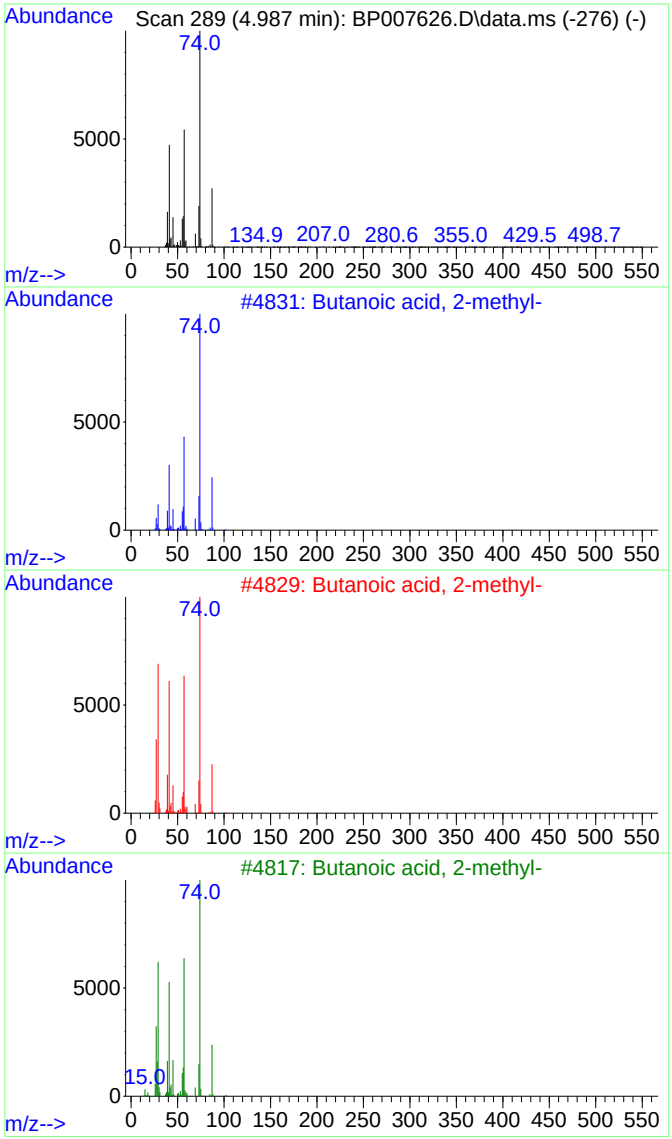
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP101421.M
Quant Title : SVOA CALIBRATION

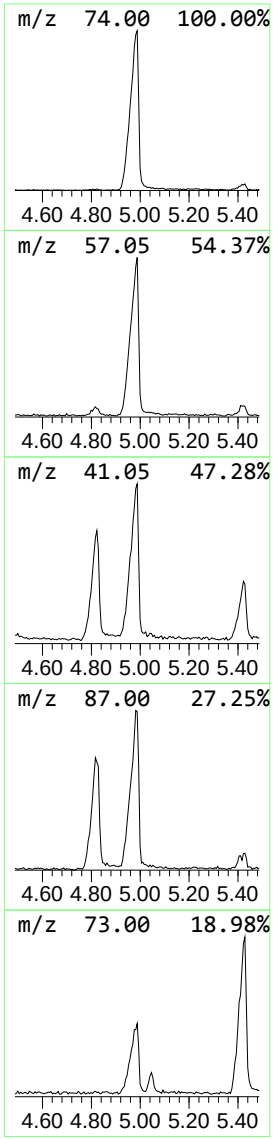
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butanoic acid, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	6.45 ng/ul	381265	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	90
2	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	78
3	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	78
4	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	64
5	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	56





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Data File : BP007626.D
Acq On : 23 Oct 2021 12:43
Operator : CG/JU
Sample : M4262-13
Misc :
ALS Vial : 86 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BFYA4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP101421.M
Quant Title : SVOA CALIBRATION

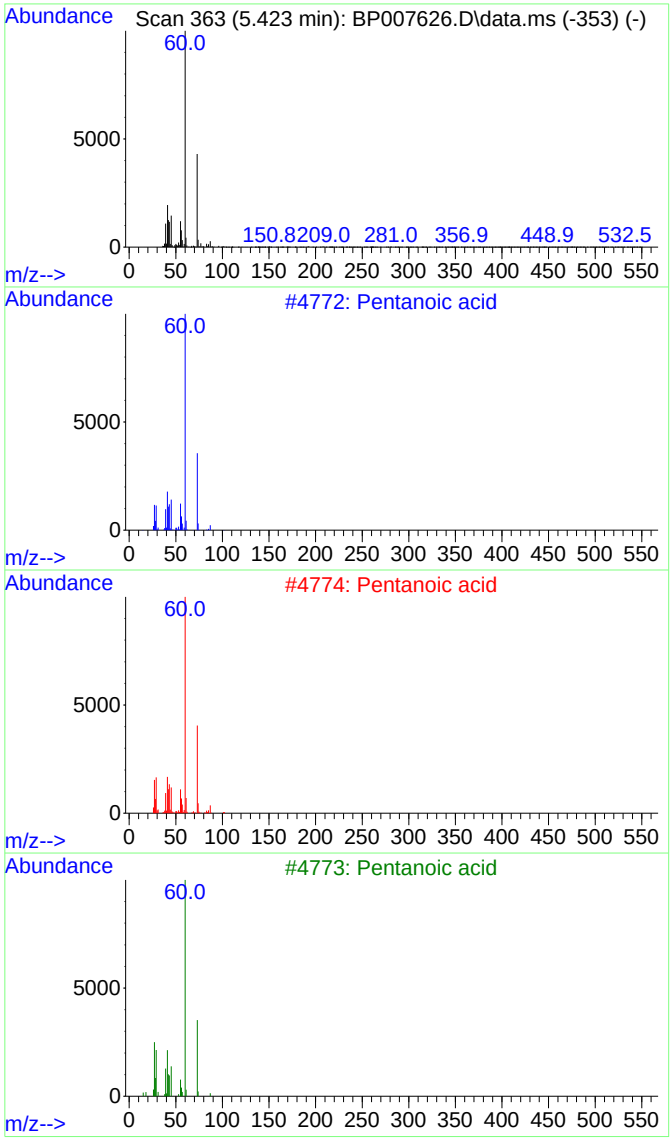
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

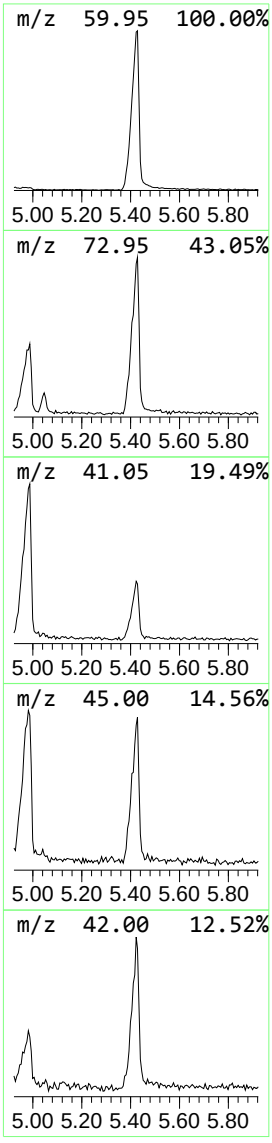
****

Peak Number 5 Pentanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.423	4.29 ng/ul	253492	1,4-Dichlorobenzene-d4	7.946

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	Butanoic acid	88	C4H8O2	000107-92-6	78
5	Butanoic acid	88	C4H8O2	000107-92-6	78





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Data File : BP007626.D
Acq On : 23 Oct 2021 12:43
Operator : CG/JU
Sample : M4262-13
Misc :
ALS Vial : 86 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BFYA4

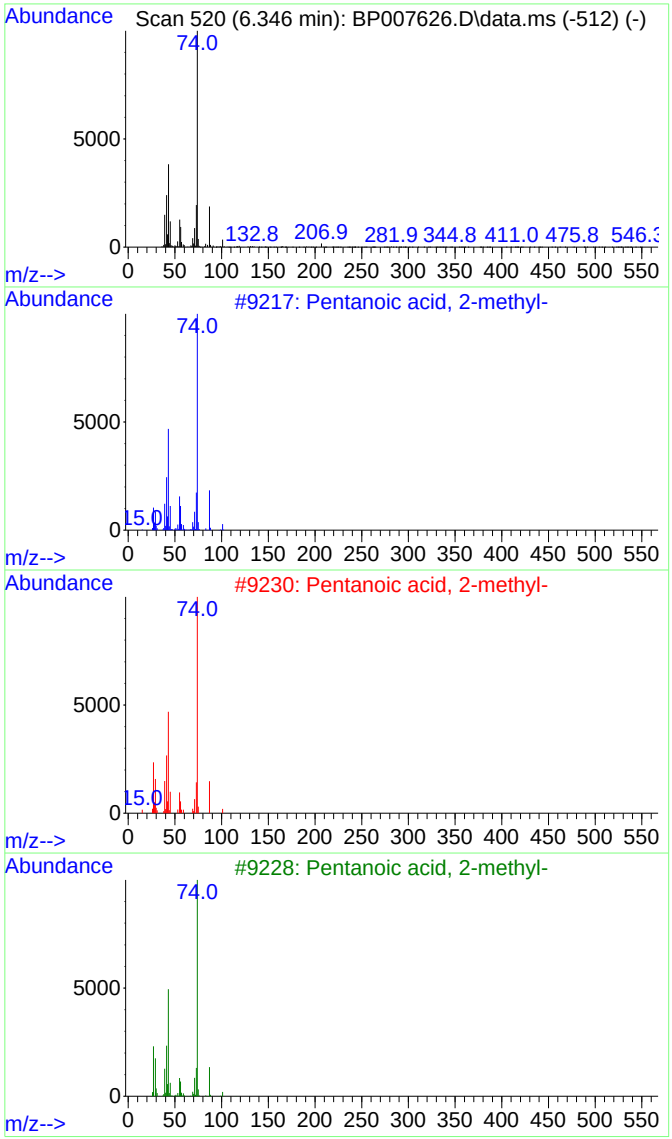
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP101421.M
Quant Title : SVOA CALIBRATION

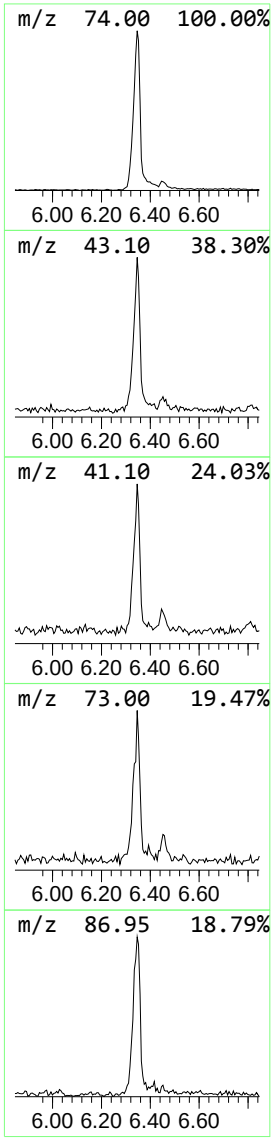
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Pentanoic acid, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.346	3.16 ng/ul	186537	1,4-Dichlorobenzene-d4	7.946

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	78
3	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	72
4	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	64
5	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102121\
Data File : BP007626.D
Acq On : 23 Oct 2021 12:43
Operator : CG/JU
Sample : M4262-13
Misc :
ALS Vial : 86 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BFYA4

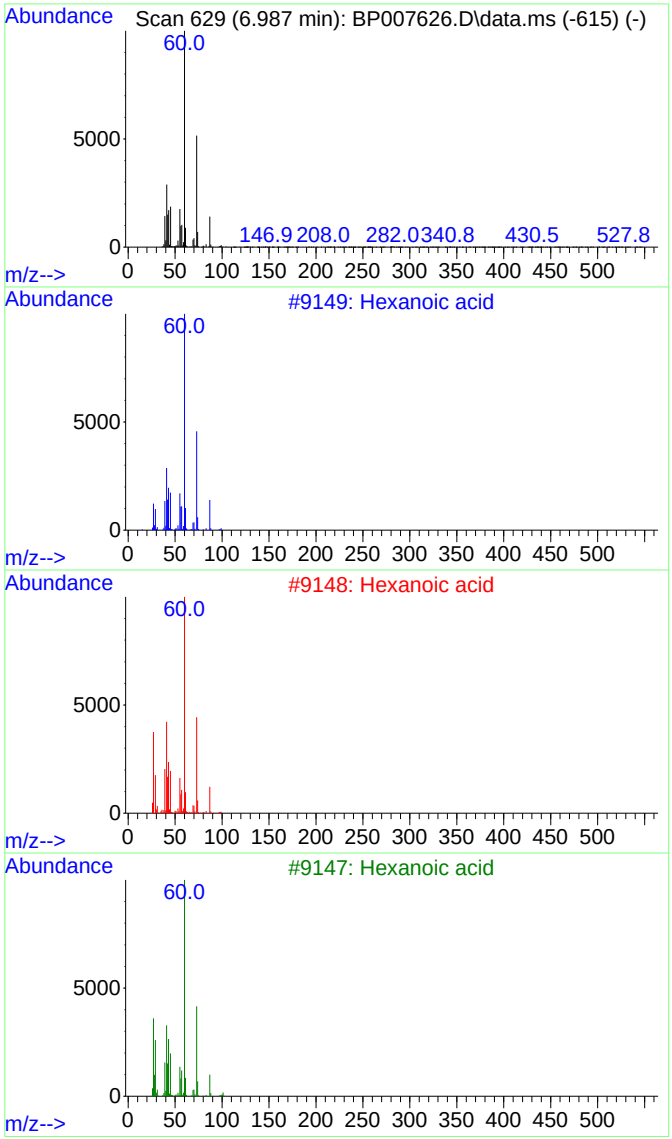
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP101421.M
Quant Title : SVOA CALIBRATION

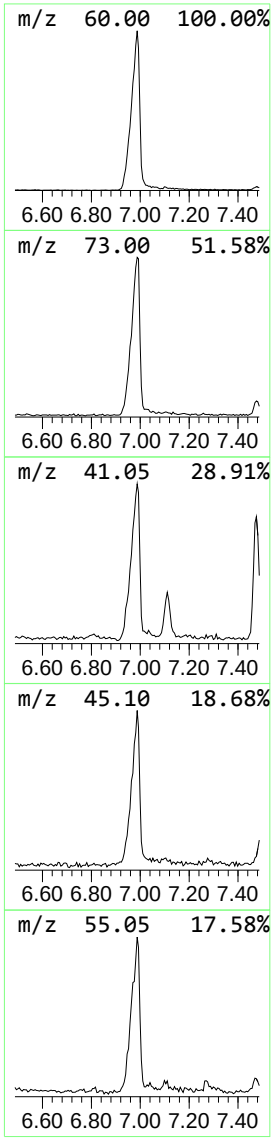
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Hexanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.987	9.01 ng/ul	532139	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid	116	C6H12O2	000142-62-1	90
2	Hexanoic acid	116	C6H12O2	000142-62-1	90
3	Hexanoic acid	116	C6H12O2	000142-62-1	83
4	Hexanoic acid	116	C6H12O2	000142-62-1	78
5	Pentanoic acid	102	C5H10O2	000109-52-4	72





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Data File : BP007626.D
Acq On : 23 Oct 2021 12:43
Operator : CG/JU
Sample : M4262-13
Misc :
ALS Vial : 86 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BFYA4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP101421.M
Quant Title : SVOA CALIBRATION

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

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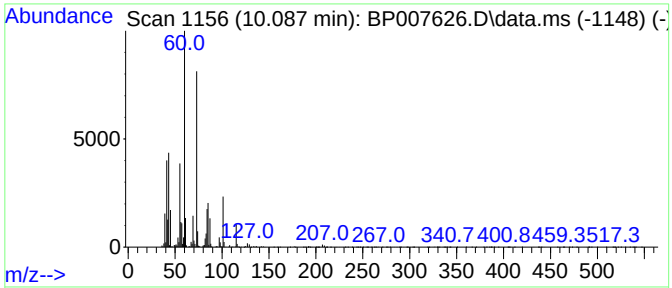
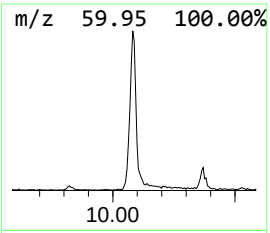
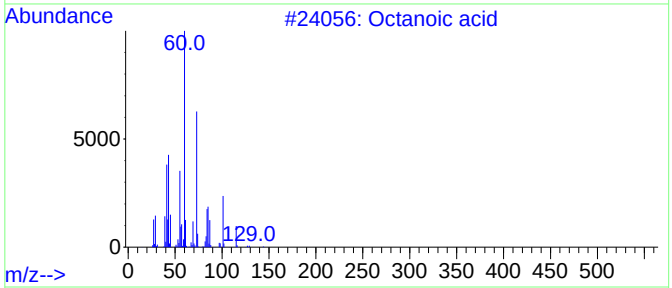
Peak Number 8 Octanoic acid Concentration Rank 7

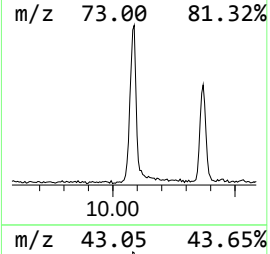
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.087	3.06 ng/ul	259512	Naphthalene-d8	10.752

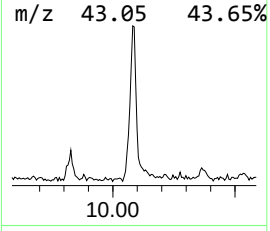
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	98
2	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	91
3	Octanoic acid	144	C8H16O2	000124-07-2	91
4	Octanoic acid	144	C8H16O2	000124-07-2	90
5	Octanoic acid	144	C8H16O2	000124-07-2	64

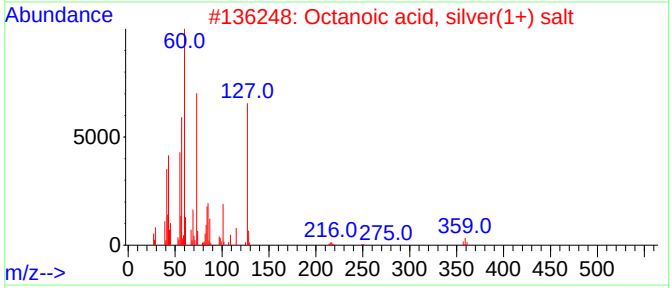


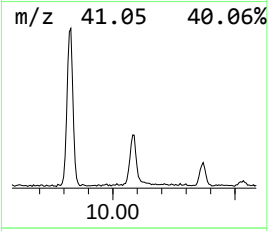


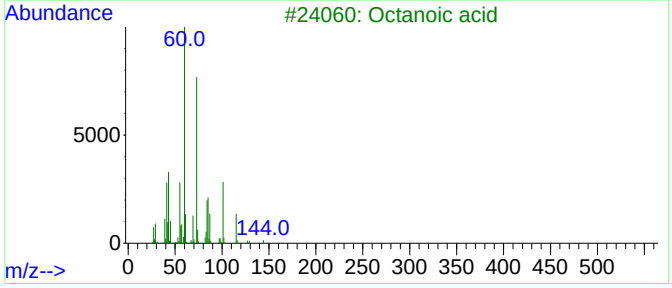


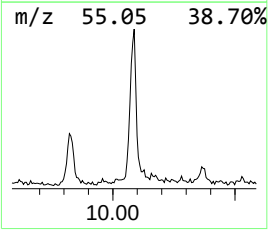












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102121\
Data File : BP007626.D
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Operator : CG/JU
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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,...	3.687	2.6	ng/ul	155392	1	7.946	1181830	20.0
Butanoic acid	4.023	3.8	ng/ul	221717	1	7.946	1181830	20.0
Butanoic acid, ...	4.823	5.0	ng/ul	298301	1	7.946	1181830	20.0
Butanoic acid, ...	4.987	6.5	ng/ul	381265	1	7.946	1181830	20.0
Pentanoic acid	5.423	4.3	ng/ul	253492	1	7.946	1181830	20.0
Pentanoic acid,...	6.346	3.2	ng/ul	186537	1	7.946	1181830	20.0
Hexanoic acid	6.987	9.0	ng/ul	532139	1	7.946	1181830	20.0
Octanoic acid	10.087	3.1	ng/ul	259512	2	10.752	1696180	20.0