LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042523\
Data File : BM039636.D
Acq On : 25 Apr 2023 12:29
Operator : CG/JU
Sample : 02433-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BHE48

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_M\Methods\SFAM-EPA-BM041823.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BM039636.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.172	18	23	27	rBV	282595	402533	1.77%	0.534%
2	3.537	82	85	95	rBV2	23044	48269	0.21%	0.064%
3	3.637	100	102	120	rBV	174010	320174	1.41%	0.424%
4	3.954	153	156	162	rVB2	25716	36657	0.16%	0.049%
5	4.490	240	247	269	rBV	15677757	22735197	100.00%	30.137%
6	4.707	276	284	293	rBV	133517	261261	1.15%	0.346%
7	4.848	302	308	320	rVB	79472	157004	0.69%	0.208%
8	5.313	383	387	393	rBV4	13435	33086	0.15%	0.044%
9	6.243	538	545	558	rBV	101202	215925	0.95%	0.286%
10	6.878	646	653	662	rBV	143408	299758	1.32%	0.397%
11	6.995	668	673	691	rVB	125481	294341	1.29%	0.390%
12	7.142	692	698	714	rVV	696257	1158769	5.10%	1.536%
13	7.266	714	719	726	rVV	36436	60742	0.27%	0.081%
14	7.342	726	732	743	rVV	633881	1070437	4.71%	1.419%
15	7.437	744	748	761	rVB2	25810	57494	0.25%	0.076%
16	7.807	800	811	821	rBV2	858034	1639329	7.21%	2.173%
17	8.066	850	855	864	rVB6	12340	29957	0.13%	0.040%
18	8.536	929	935	940	rBV	464507	794720	3.50%	1.053%
19	8.595	940	945	966	rVB	687809	1337120	5.88%	1.772%
20	8.984	1004	1011	1031	rBV	772844	1423850	6.26%	1.887%
21	9.331	1064	1070	1074	rBV	15323	34283	0.15%	0.045%
22	9.701	1126	1133	1149	rBV	600823	1154815	5.08%	1.531%
23	9.995	1176	1183	1196	rBV4	46445	173133	0.76%	0.229%
24	10.254	1220	1227	1249	rBV	676028	1537702	6.76%	2.038%
25	10.613	1281	1288	1306	rBV	1200090	2067222	9.09%	2.740%
26	10.772	1308	1315	1337	rBV	498808	1161367	5.11%	1.539%
27	11.225	1386	1392	1404	rBV	78510	277104	1.22%	0.367%
28	12.148	1543	1549	1556	rBV3	17204	43332	0.19%	0.057%
29	12.295	1569	1574	1589	rBV	79101	246790	1.09%	0.327%
30	13.336	1745	1751	1760	rBV	75896	150824	0.66%	0.200%
31	13.883	1836	1844	1857	rBV	2025372	2879310	12.66%	3.817%
32	13.995	1860	1863	1873	rVB10	12114	23088	0.10%	0.031%
33	14.160	1883	1891	1903	rBV	2274646	3363091	14.79%	4.458%
34	14.324	1912	1919	1933	rBV2	44654	133245	0.59%	0.177%
35	14.466	1936	1943	1956	rBV2	1898347	3107038	13.67%	4.119%
36	14.777	1991	1996	2001	rBV6	20376	53073	0.23%	0.070%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042523\
Data File : BM039636.D
Acq On : 25 Apr 2023 12:29
Operator : CG/JU
Sample : 02433-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BHE48

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_M\Methods\SFAM-EPA-BM041823.MA.M
Title : SVOA CALIBRATION

37	15.218	2066	2071	2084	rBV	113881	268157	1.18%	0.355%
38	15.460	2106	2112	2127	rBV	2833364	4166480	18.33%	5.523%
39	15.607	2131	2137	2150	rVV	233986	450953	1.98%	0.598%
40	15.701	2150	2153	2169	rVB9	21827	57303	0.25%	0.076%
41	15.836	2169	2176	2189	rBV	129363	223375	0.98%	0.296%
42	16.765	2326	2334	2342	rBV5	9590	31717	0.14%	0.042%
43	17.218	2405	2411	2422	rBV	2127823	3028802	13.32%	4.015%
44	17.318	2422	2428	2436	rBV	2968292	4297725	18.90%	5.697%
45	17.671	2483	2488	2497	rBV	80548	145640	0.64%	0.193%
46	18.118	2560	2564	2573	rBV2	51187	101843	0.45%	0.135%
47	19.183	2741	2745	2750	rVB3	31479	46508	0.20%	0.062%
48	19.259	2753	2758	2762	rBV	30689	50110	0.22%	0.066%
49	19.400	2779	2782	2792	rBV5	27247	57386	0.25%	0.076%
50	19.542	2802	2806	2810	rBV4	42628	55578	0.24%	0.074%
51	19.618	2813	2819	2837	rBV	3503187	4827429	21.23%	6.399%
52	21.130	3072	3076	3083	rBV5	52741	106670	0.47%	0.141%
53	21.418	3120	3125	3134	rBV	1835336	2532836	11.14%	3.357%
54	21.500	3136	3139	3146	rVV	122863	225323	0.99%	0.299%
55	23.624	3493	3500	3517	rBV2	1773691	3704705	16.30%	4.911%
56	23.777	3520	3526	3539	rVB2	1080021	2278672	10.02%	3.021%

Sum of corrected areas: 75439252

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Data File : BM039636.D
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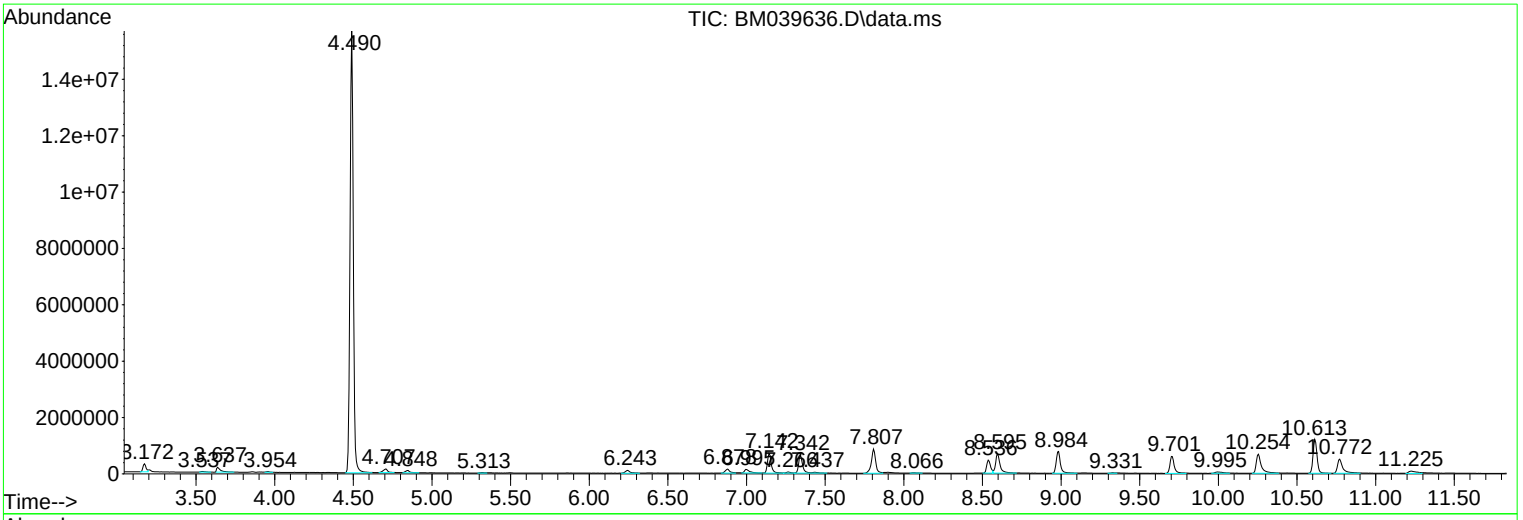
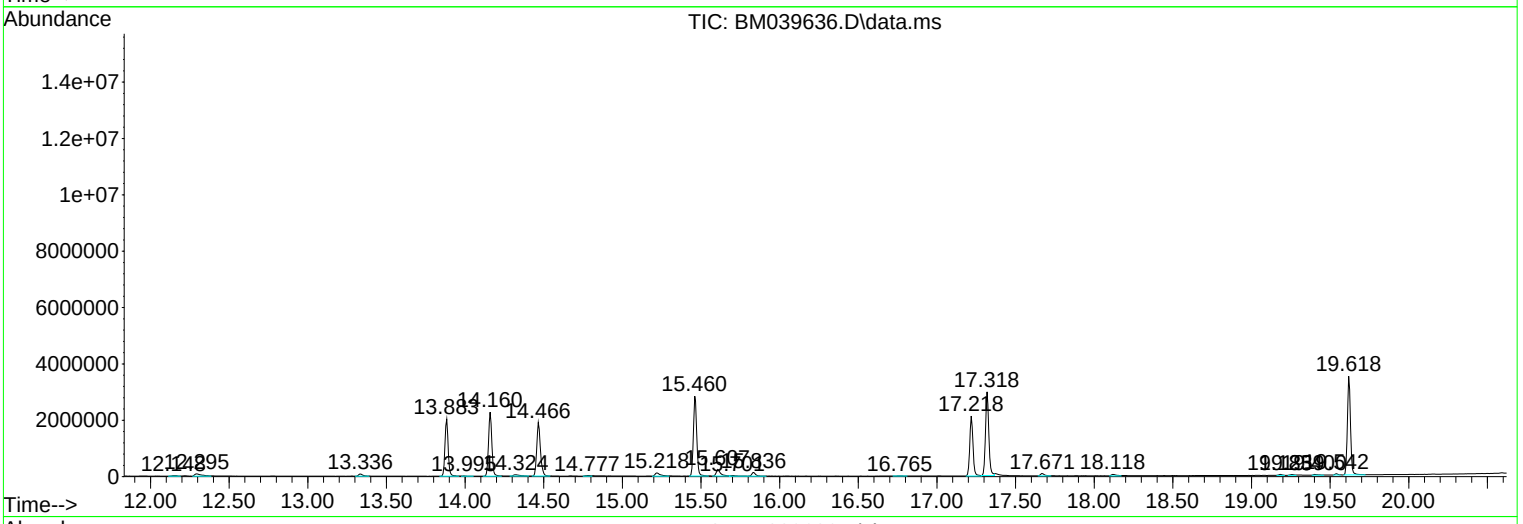
Sample : 02433-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

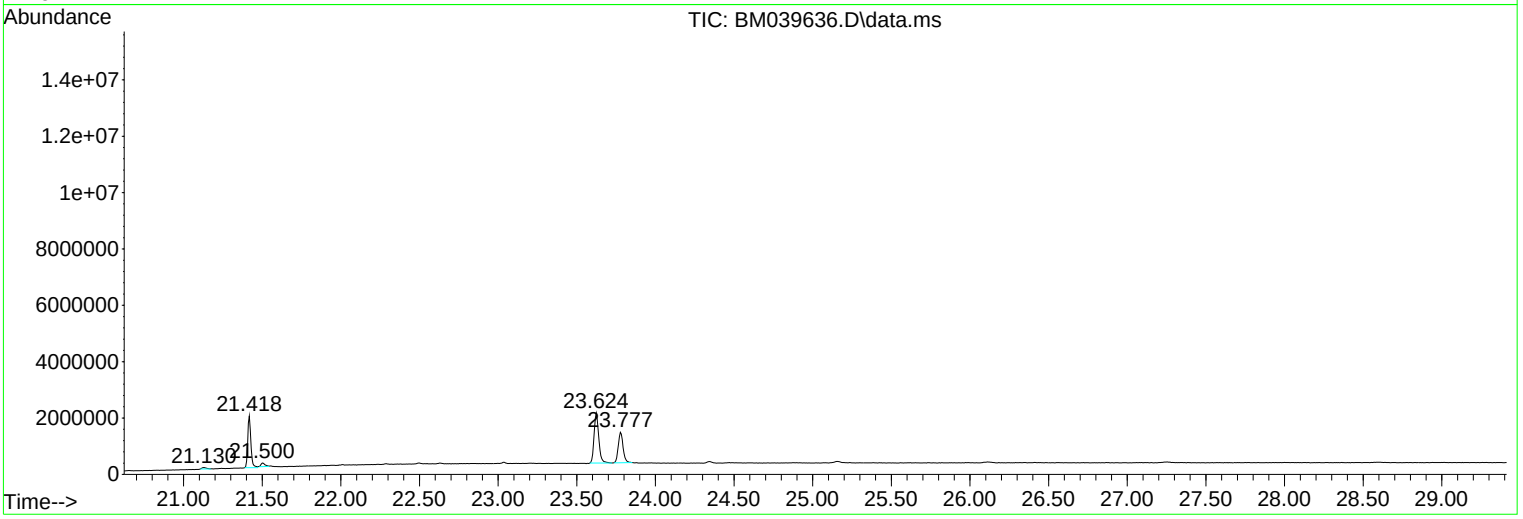
Instrument :
BNA_M
ClientSampleId :
BHE48

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042523\
Data File : BM039636.D
Acq On : 25 Apr 2023 12:29
Operator : CG/JU
Sample : 02433-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BHE48

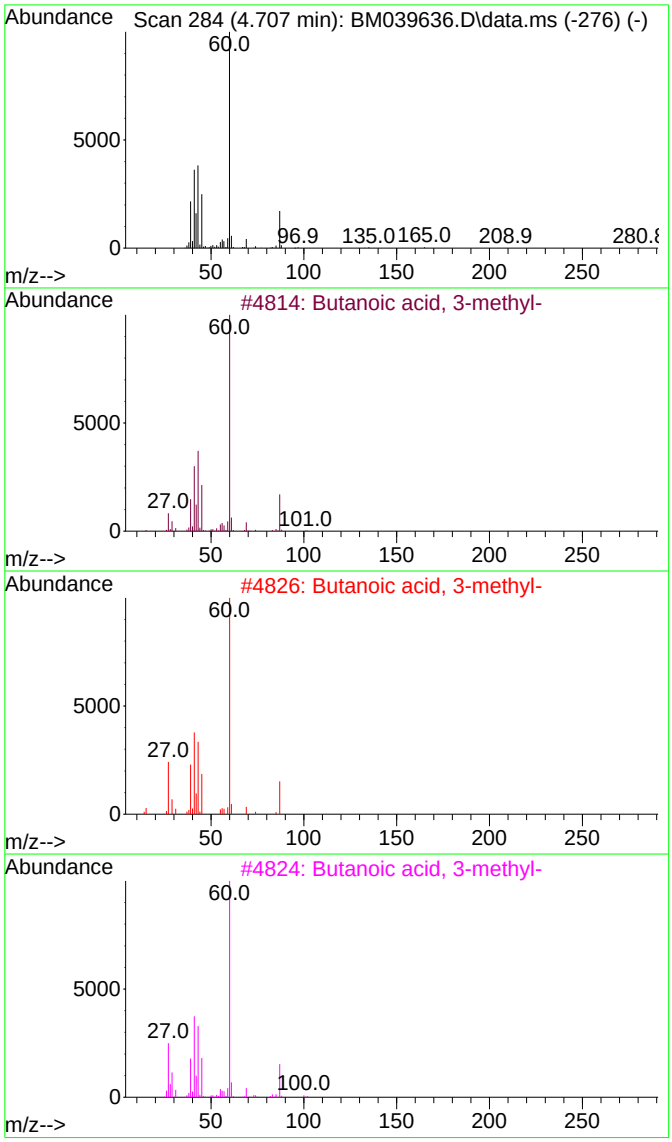
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

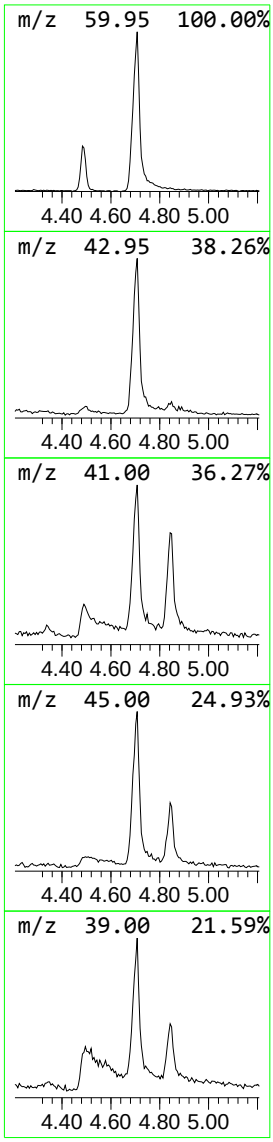
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butanoic acid, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.707	3.19 ng/ul	261261	1,4-Dichlorobenzene-d4	7.807

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	78
4	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	72
5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	56





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042523\
Data File : BM039636.D
Acq On : 25 Apr 2023 12:29
Operator : CG/JU
Sample : 02433-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BHE48

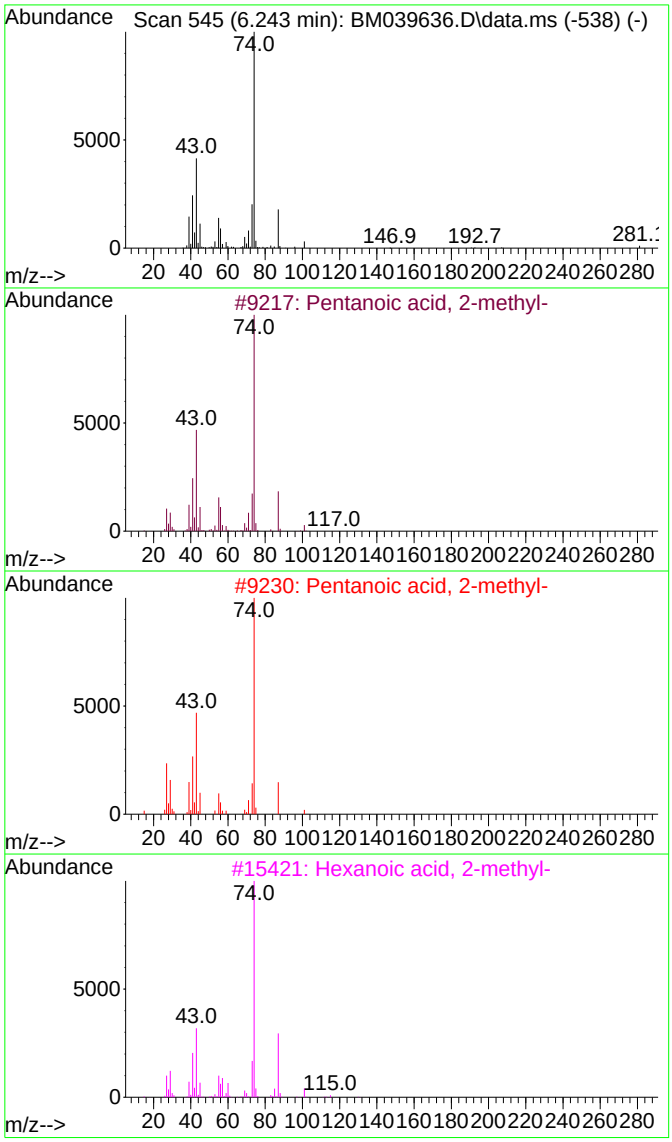
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

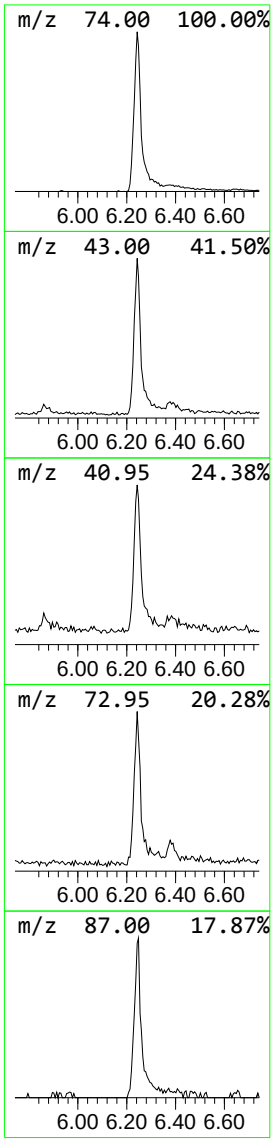
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentanoic acid, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.243	2.63 ng/ul	215925	1,4-Dichlorobenzene-d4	7.807

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	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	72
4	Octanoic acid, 2-methyl-	158	C9H18O2	003004-93-1	64
5	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	56





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042523\
Data File : BM039636.D
Acq On : 25 Apr 2023 12:29
Operator : CG/JU
Sample : 02433-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BHE48

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

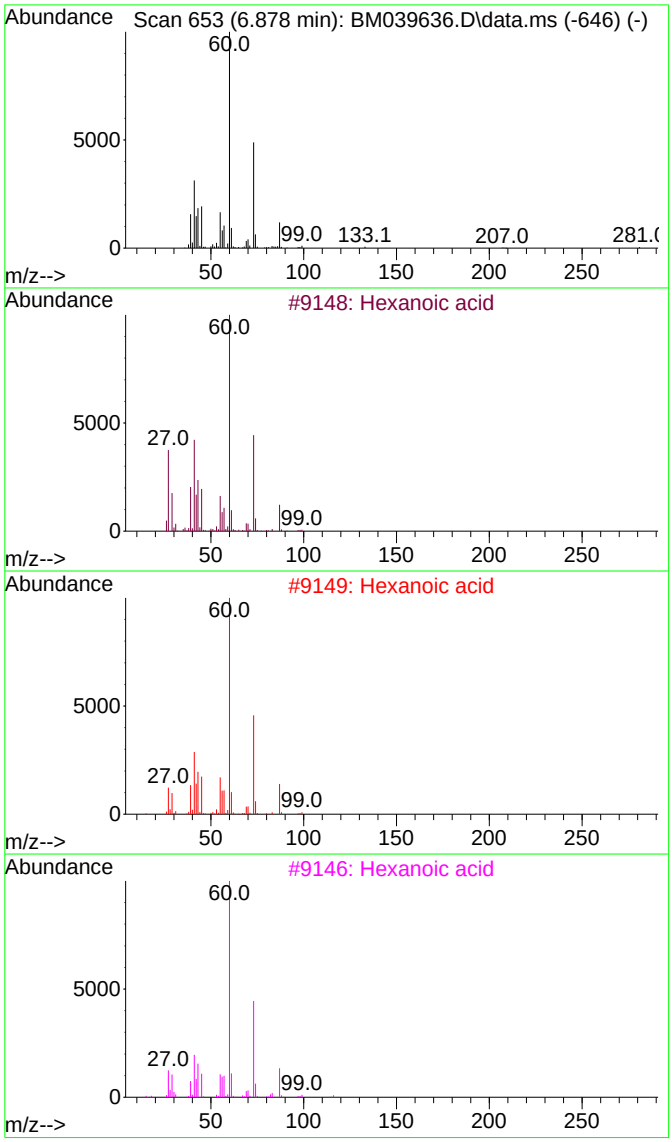
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

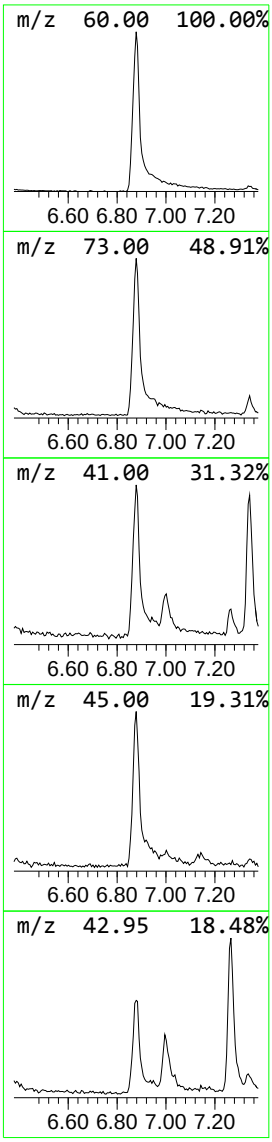
****

Peak Number 4 Hexanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.878	3.66 ng/ul	299758	1,4-Dichlorobenzene-d4	7.807

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	78
4	Hexanoic acid	116	C6H12O2	000142-62-1	78
5	Pentanoic acid	102	C5H10O2	000109-52-4	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042523\
Data File : BM039636.D
Acq On : 25 Apr 2023 12:29
Operator : CG/JU
Sample : 02433-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BHE48

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

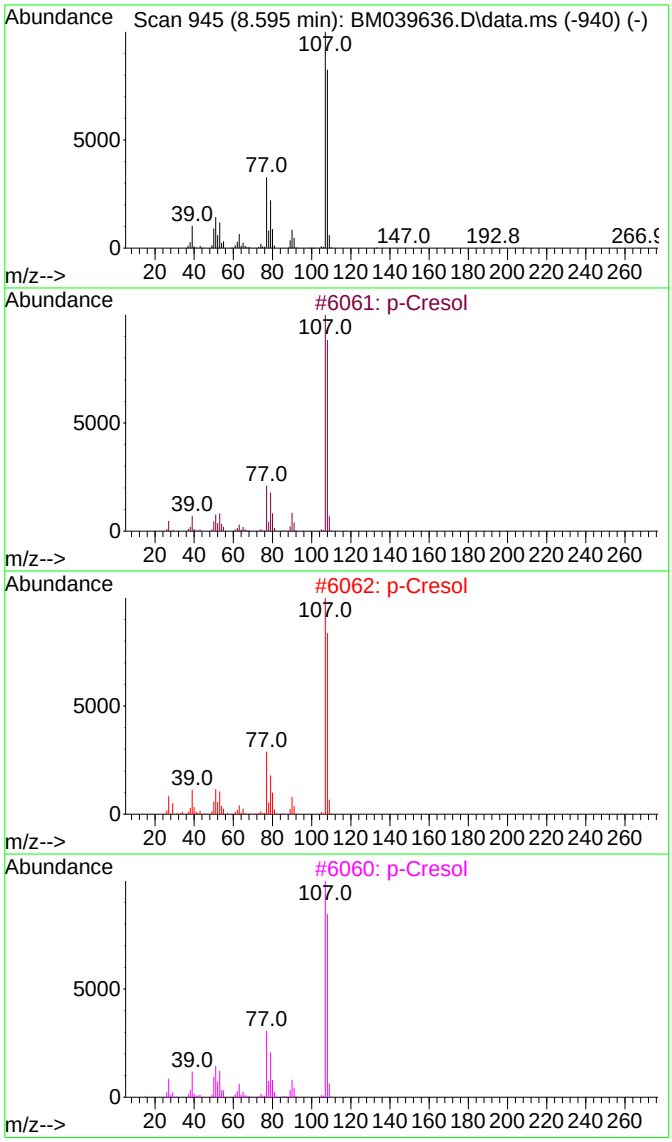
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

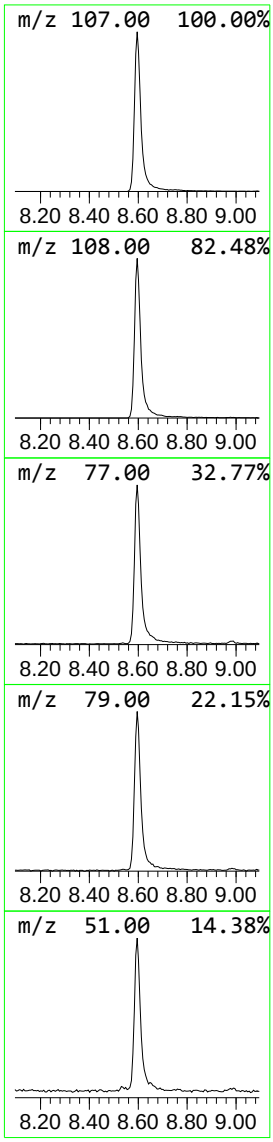
****

Peak Number 5 p-Cresol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.595	16.31 ng/ul	1337120	1,4-Dichlorobenzene-d4	7.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Cresol	108	C7H8O	000106-44-5	97
2	p-Cresol	108	C7H8O	000106-44-5	97
3	p-Cresol	108	C7H8O	000106-44-5	96
4	p-Cresol	108	C7H8O	000106-44-5	95
5	Phenol, 3-methyl-	108	C7H8O	000108-39-4	90





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Acq On : 25 Apr 2023 12:29
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Sample : 02433-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BHE48

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

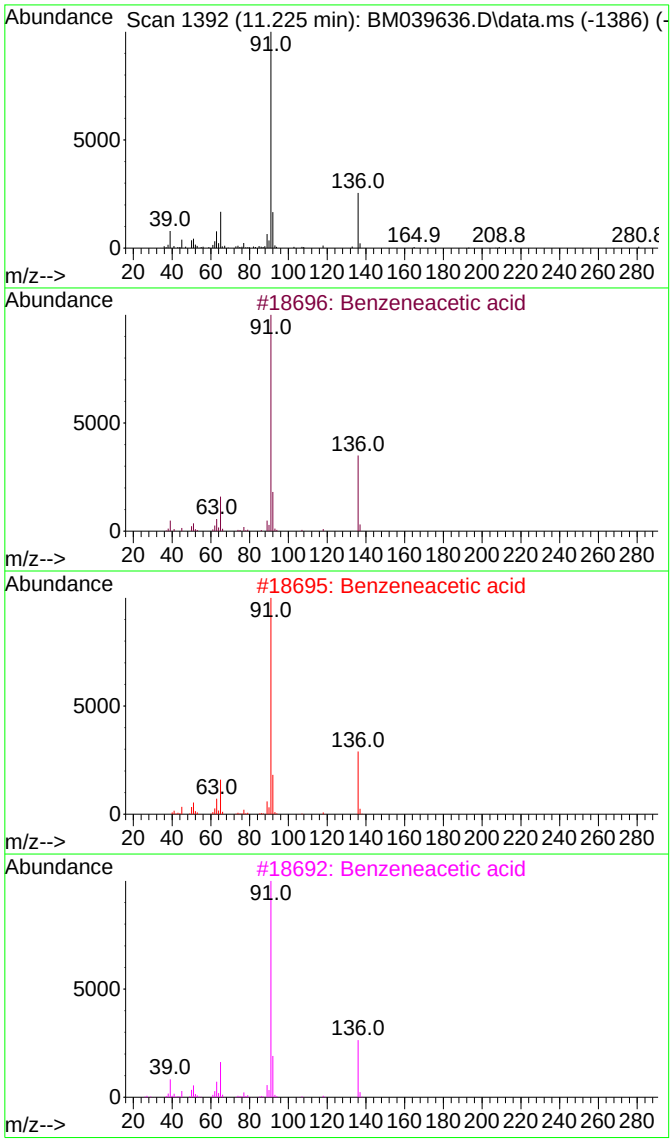
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

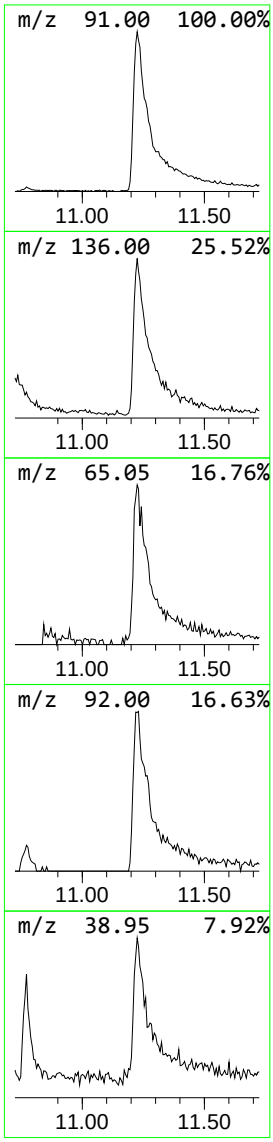
****

Peak Number 6 Benzeneacetic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.225	2.68 ng/ul	277104	Naphthalene-d8	10.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetic acid	136	C8H8O2	000103-82-2	93
2	Benzeneacetic acid	136	C8H8O2	000103-82-2	93
3	Benzeneacetic acid	136	C8H8O2	000103-82-2	90
4	Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	78
5	Benzeneacetic acid	136	C8H8O2	000103-82-2	64





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Operator : CG/JU
Sample : 02433-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BHE48

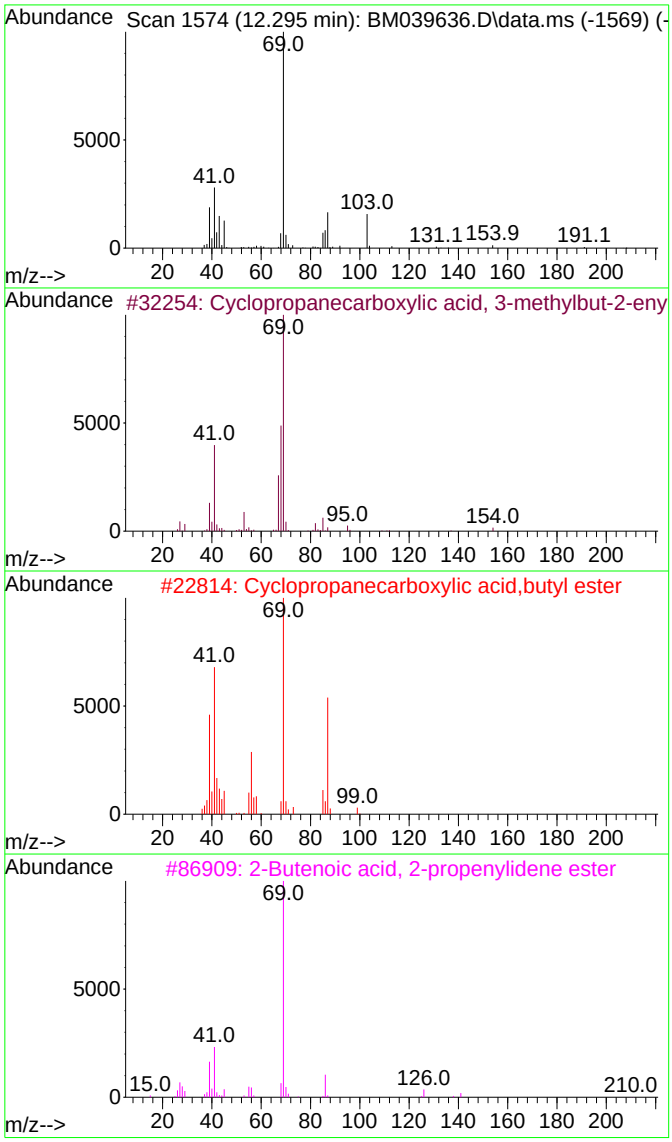
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

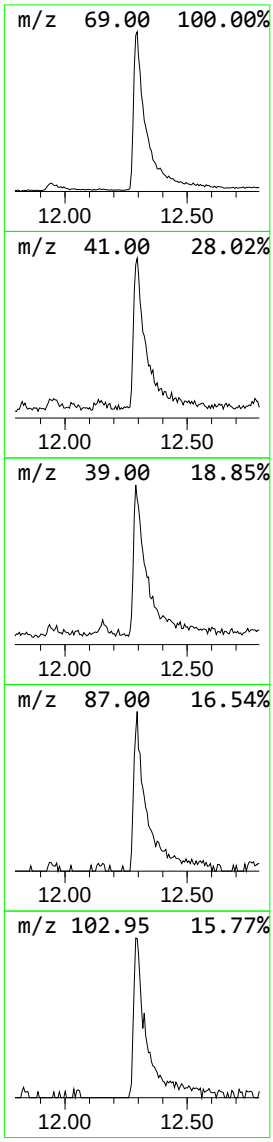
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclopropanecarboxylic acid... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.295	2.39 ng/ul	246790	Naphthalene-d8	10.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	53
2	Cyclopropanecarboxylic acid,buty...	142	C8H14O2	054947-39-6	45
3	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	40
4	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	39
5	3-Methyl-3-(3-hydroxy-3-methylbu...	190	C10H22O3	1000432-16-8	39





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042523\
Data File : BM039636.D
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Operator : CG/JU
Sample : 02433-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BHE48

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.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
Butanoic acid, ...	4.707	3.2	ng/ul	261261	1	7.807	1639330	20.0
Pentanoic acid,...	6.243	2.6	ng/ul	215925	1	7.807	1639330	20.0
Hexanoic acid	6.878	3.7	ng/ul	299758	1	7.807	1639330	20.0
p-Cresol	8.595	16.3	ng/ul	1337120	1	7.807	1639330	20.0
Benzeneacetic acid	11.225	2.7	ng/ul	277104	2	10.613	2067220	20.0
Cyclopropanecar...	12.295	2.4	ng/ul	246790	2	10.613	2067220	20.0