LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092322\
Data File : BM036674.D
Acq On : 23 Sep 2022 13:15
Operator : CG/JU
Sample : N4595-06DL 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CB8H4DL

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-BM091522.M
Title : SVOA CALIBRATION

Signal : TIC: BM036674.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.122	3	6	36	rVB	4237700	5873973	91.44%	6.810%
2	3.393	49	52	54	rBV2	22347	24473	0.38%	0.028%
3	3.428	54	58	69	rVB	560007	733860	11.42%	0.851%
4	3.681	97	101	107	rBV2	52774	72362	1.13%	0.084%
5	3.828	124	126	140	rBV	186825	292430	4.55%	0.339%
6	4.057	162	165	175	rVB	27401	49077	0.76%	0.057%
7	4.151	177	181	187	rBV	34653	50806	0.79%	0.059%
8	4.234	191	195	200	rBV	128889	167123	2.60%	0.194%
9	4.610	253	259	265	rVB2	123123	198753	3.09%	0.230%
10	5.104	338	343	350	rBV	64496	96268	1.50%	0.112%
11	5.304	370	377	383	rBV	31082	51685	0.80%	0.060%
12	5.581	418	424	425	rBV6	8756	15499	0.24%	0.018%
13	5.704	439	445	450	rBV10	7606	13405	0.21%	0.016%
14	5.798	457	461	466	rVB6	6895	11636	0.18%	0.013%
15	5.939	480	485	487	rVB6	9147	14370	0.22%	0.017%
16	6.092	506	511	515	rVB4	8260	14731	0.23%	0.017%
17	6.281	538	543	548	rVB	18212	29773	0.46%	0.035%
18	6.598	592	597	601	rVB8	10326	20434	0.32%	0.024%
19	7.169	686	694	701	rBV	243168	407259	6.34%	0.472%
20	7.345	717	724	733	rBV	820912	1300660	20.25%	1.508%
21	7.463	739	744	749	rVB5	8691	16347	0.25%	0.019%
22	7.545	749	758	768	rVV	804154	1288392	20.06%	1.494%
23	7.634	770	773	778	rVV7	9435	14991	0.23%	0.017%
24	7.875	808	814	819	rBV10	7574	14849	0.23%	0.017%
25	8.016	831	838	846	rVV	1862493	2947383	45.88%	3.417%
26	8.086	846	850	862	rVB3	24741	68631	1.07%	0.080%
27	8.481	912	917	923	rVB7	9824	17857	0.28%	0.021%
28	8.575	923	933	934	rBV9	7352	16049	0.25%	0.019%
29	8.722	947	958	966	rBV	732879	1203516	18.74%	1.395%
30	8.822	969	975	983	rVB9	14438	45301	0.71%	0.053%
31	8.928	989	993	996	rBV6	7503	10605	0.17%	0.012%
32	9.004	1000	1006	1018	rVV	809310	1366596	21.27%	1.584%
33	9.128	1022	1027	1030	rVV	37728	54960	0.86%	0.064%
34	9.180	1030	1036	1044	rVB	991961	1573350	24.49%	1.824%
35	9.292	1052	1055	1060	rVB3	12060	19669	0.31%	0.023%
36	9.392	1066	1072	1079	rVB8	20783	41237	0.64%	0.048%

LSC Area Percent Report

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Operator : CG/JU
Sample : N4595-06DL 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CB8H4DL

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-BM091522.M
Title : SVOA CALIBRATION

37	9.545	1091	1098	1104	rBV6	34029	73761	1.15%	0.086%
38	9.616	1104	1110	1115	rVV5	34890	81656	1.27%	0.095%
39	9.663	1115	1118	1125	rVB5	28528	49078	0.76%	0.057%
40	9.780	1133	1138	1141	rVB7	10601	17299	0.27%	0.020%
41	9.833	1141	1147	1153	rBV7	12523	27257	0.42%	0.032%
42	9.904	1153	1159	1173	rVB	730893	1183703	18.43%	1.372%
43	10.051	1179	1184	1191	rVB9	17434	29197	0.45%	0.034%
44	10.239	1212	1216	1224	rVB10	10323	22107	0.34%	0.026%
45	10.316	1224	1229	1232	rBV6	13382	23949	0.37%	0.028%
46	10.380	1232	1240	1244	rVV3	37524	84557	1.32%	0.098%
47	10.445	1244	1251	1272	rVB	1296565	2261267	35.20%	2.622%
48	10.616	1275	1280	1288	rVB	14657	35412	0.55%	0.041%
49	10.757	1297	1304	1309	rBV	33994	63465	0.99%	0.074%
50	10.827	1309	1316	1323	rVV	2725929	4461478	69.45%	5.173%
51	10.880	1323	1325	1331	rVB7	11138	14838	0.23%	0.017%
52	10.963	1331	1339	1352	rBV	712002	1236779	19.25%	1.434%
53	11.080	1354	1359	1363	rVB8	12856	24087	0.37%	0.028%
54	11.133	1363	1368	1373	rBV9	12350	26381	0.41%	0.031%
55	11.186	1374	1377	1382	rVB6	12748	19924	0.31%	0.023%
56	11.416	1412	1416	1422	rVB8	16221	31396	0.49%	0.036%
57	11.621	1443	1451	1453	rBV9	21040	42492	0.66%	0.049%
58	11.798	1476	1481	1486	rBV8	14159	24213	0.38%	0.028%
59	12.033	1517	1521	1526	rBV2	33953	54270	0.84%	0.063%
60	12.110	1526	1534	1538	rVV7	34503	74982	1.17%	0.087%
61	12.163	1539	1543	1554	rVB4	37876	72119	1.12%	0.084%
62	12.321	1564	1570	1577	rBV	425098	670703	10.44%	0.778%
63	12.427	1581	1588	1595	rBV3	80996	183218	2.85%	0.212%
64	12.545	1603	1608	1611	rBV4	19558	31261	0.49%	0.036%
65	12.633	1617	1623	1629	rVB	159790	251945	3.92%	0.292%
66	12.698	1631	1634	1640	rVB8	12332	24140	0.38%	0.028%
67	12.780	1644	1648	1649	rBV3	13353	16688	0.26%	0.019%
68	12.810	1650	1653	1658	rVB2	29853	48121	0.75%	0.056%
69	13.027	1682	1690	1696	rBV2	25271	69252	1.08%	0.080%
70	13.198	1715	1719	1725	rBV8	22209	44219	0.69%	0.051%
71	13.380	1746	1750	1754	rBV7	17130	32773	0.51%	0.038%
72	13.545	1776	1778	1783	rVB4	24477	33643	0.52%	0.039%
73	13.686	1799	1802	1807	rBV	23499	32079	0.50%	0.037%
74	13.739	1808	1811	1816	rVB2	28731	32761	0.51%	0.038%
75	14.051	1859	1864	1873	rVB	2410831	3381243	52.64%	3.920%
76	14.198	1885	1889	1895	rVB8	26212	39928	0.62%	0.046%

LSC Area Percent Report

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Data File : BM036674.D
Acq On : 23 Sep 2022 13:15
Operator : CG/JU
Sample : N4595-06DL 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CB8H4DL

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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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM091522.M
Title : SVOA CALIBRATION

77	14.339	1906	1913	1925	rBV	2707692	4083369	63.57%	4.734%
78	14.439	1926	1930	1943	rVB2	71385	142129	2.21%	0.165%
79	14.568	1947	1952	1956	rVV2	170073	234076	3.64%	0.271%
80	14.639	1958	1964	1976	rVB	3928310	5758923	89.65%	6.677%
81	14.833	1992	1997	2005	rBV	191352	293516	4.57%	0.340%
82	15.380	2086	2090	2096	rBV	153357	228056	3.55%	0.264%
83	15.627	2126	2132	2142	rBV	3740783	5168928	80.47%	5.993%
84	15.739	2146	2151	2158	rVV	875069	1166878	18.17%	1.353%
85	15.862	2168	2172	2175	rBV3	52624	84992	1.32%	0.099%
86	16.139	2214	2219	2224	rBV	826961	1152735	17.95%	1.337%
87	16.468	2272	2275	2279	rVB	54826	64687	1.01%	0.075%
88	16.645	2298	2305	2310	rBV	491940	717122	11.16%	0.831%
89	17.380	2424	2430	2436	rBV	4570292	6423557	100.00%	7.448%
90	17.474	2441	2446	2456	rVB	3651535	5235492	81.50%	6.070%
91	18.274	2578	2582	2589	rBV	385735	571827	8.90%	0.663%
92	19.050	2711	2714	2719	rVB3	106843	131515	2.05%	0.152%
93	19.544	2794	2798	2803	rBV	238583	324813	5.06%	0.377%
94	19.762	2829	2835	2839	rBV	4010162	5584876	86.94%	6.475%
95	19.803	2839	2842	2849	rVB	303851	466430	7.26%	0.541%
96	20.756	3001	3004	3007	rBV	290830	292349	4.55%	0.339%
97	21.256	3086	3089	3094	rVB	450497	502752	7.83%	0.583%
98	21.544	3133	3138	3146	rBV	4448751	5627739	87.61%	6.525%
99	23.827	3520	3526	3533	rBV2	2051750	4031814	62.77%	4.675%
100	23.985	3547	3553	3562	rVB2	2511894	4895311	76.21%	5.676%

Sum of corrected areas: 86249837

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092322\
Data File : BM036674.D
Acq On : 23 Sep 2022 13:15
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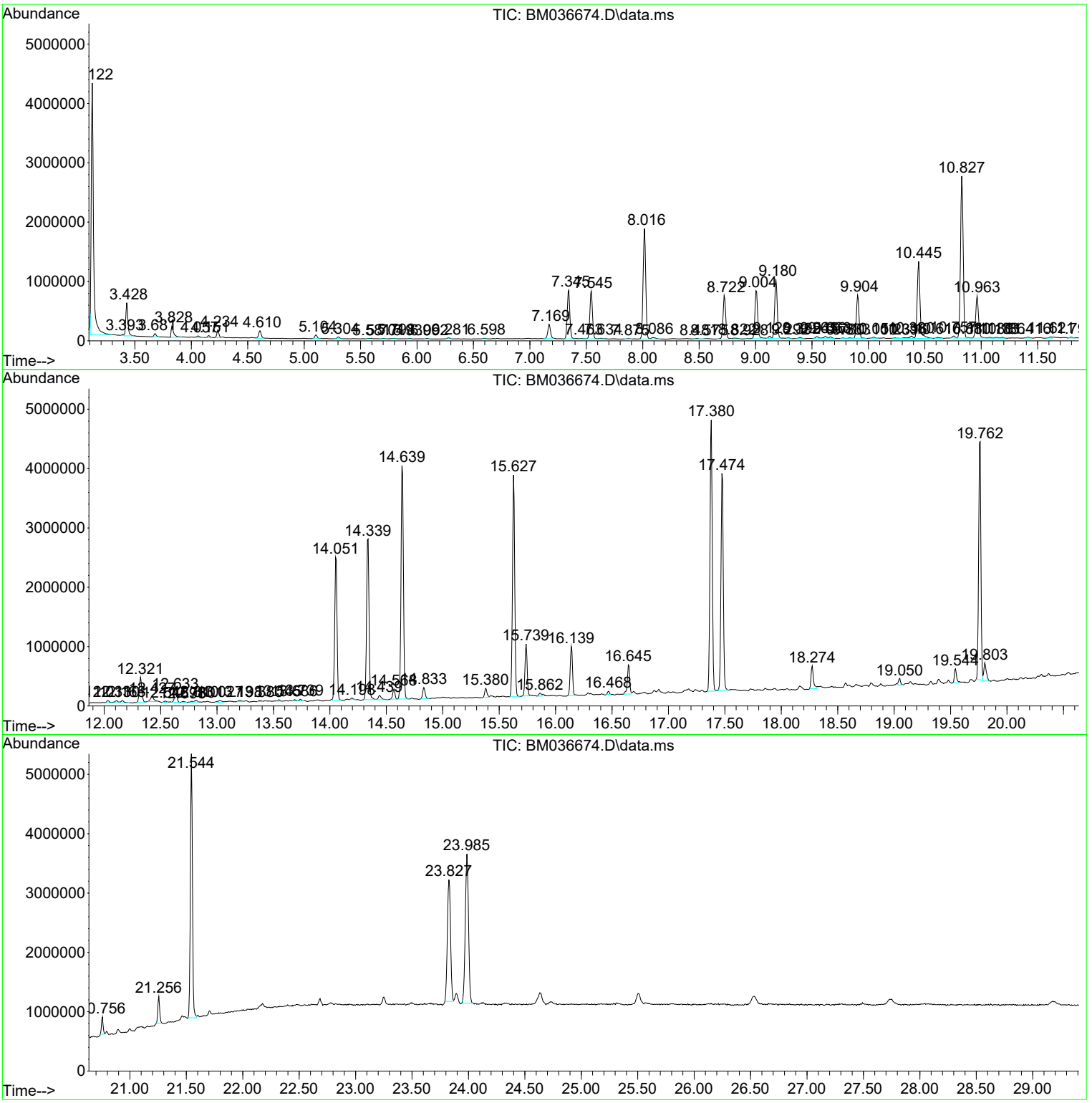
Sample : N4595-06DL 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CB8H4DL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM091522.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092322\
Data File : BM036674.D
Acq On : 23 Sep 2022 13:15
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Sample : N4595-06DL 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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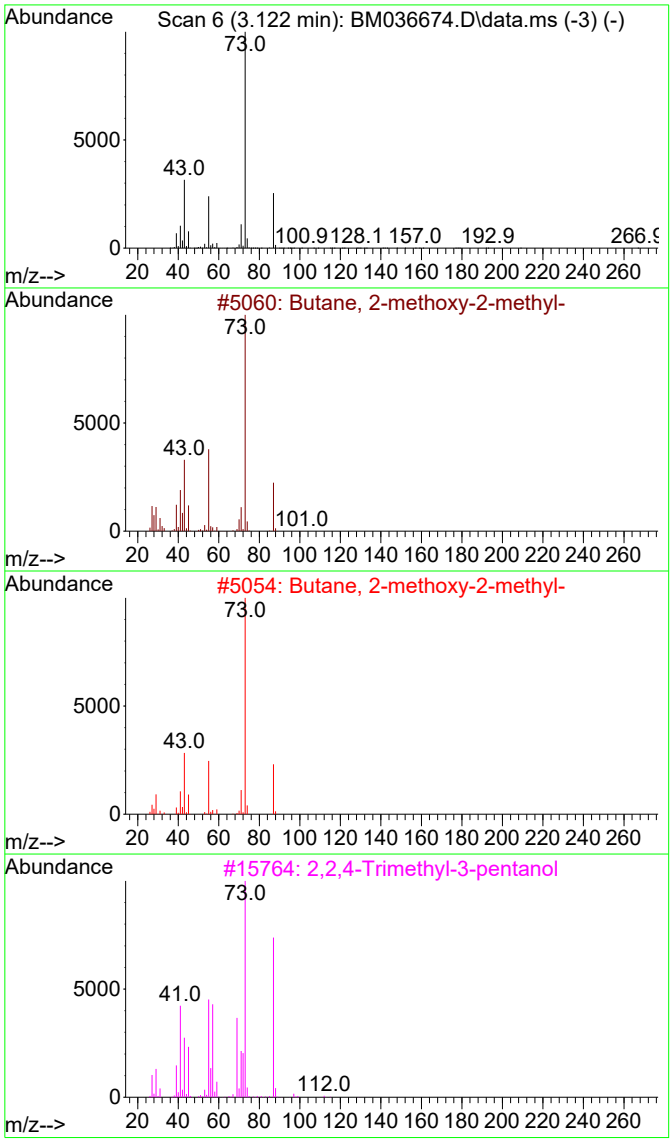
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM091522.M
Quant Title : SVOA CALIBRATION

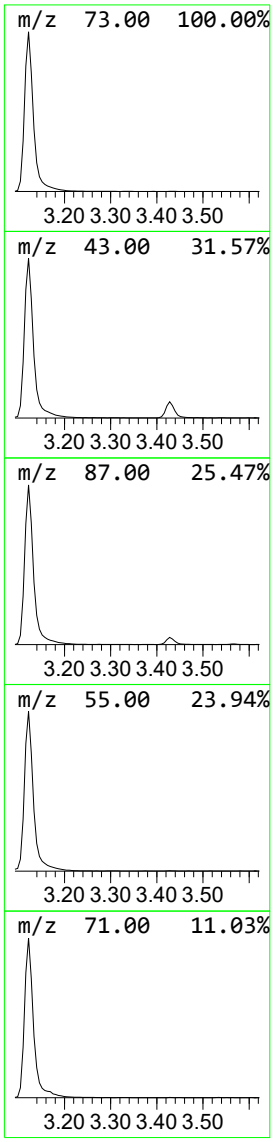
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.122	39.86 ng/ul	5873970	1,4-Dichlorobenzene-d4	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092322\
Data File : BM036674.D
Acq On : 23 Sep 2022 13:15
Operator : CG/JU
Sample : N4595-06DL 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CB8H4DL

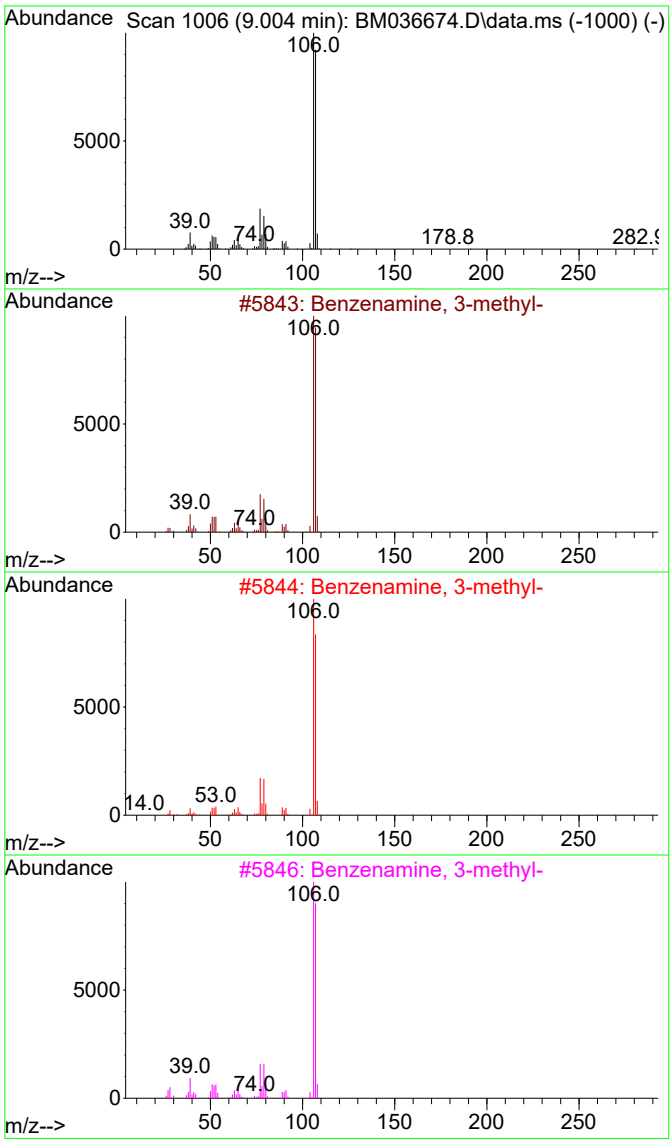
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM091522.M
Quant Title : SVOA CALIBRATION

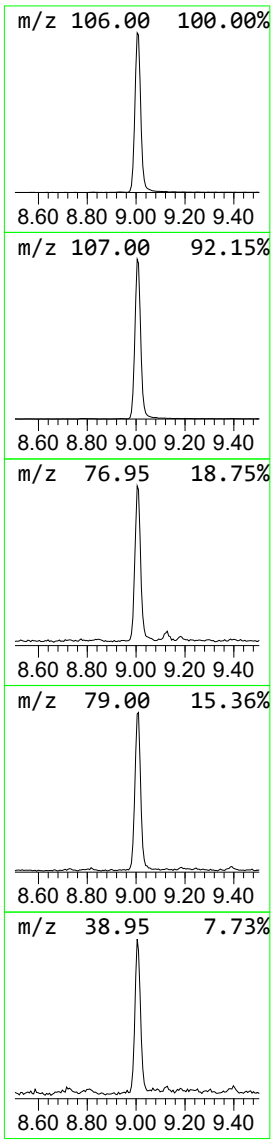
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzenamine, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.004	9.27 ng/ul	1366600	1,4-Dichlorobenzene-d4	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 3-methyl-	107	C7H9N	000108-44-1	97
2	Benzenamine, 3-methyl-	107	C7H9N	000108-44-1	97
3	Benzenamine, 3-methyl-	107	C7H9N	000108-44-1	97
4	Benzenamine, 3-methyl-	107	C7H9N	000108-44-1	95
5	o-Toluidine	107	C7H9N	000095-53-4	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092322\
Data File : BM036674.D
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Sample : N4595-06DL 2X
Misc :
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ClientSampleId :
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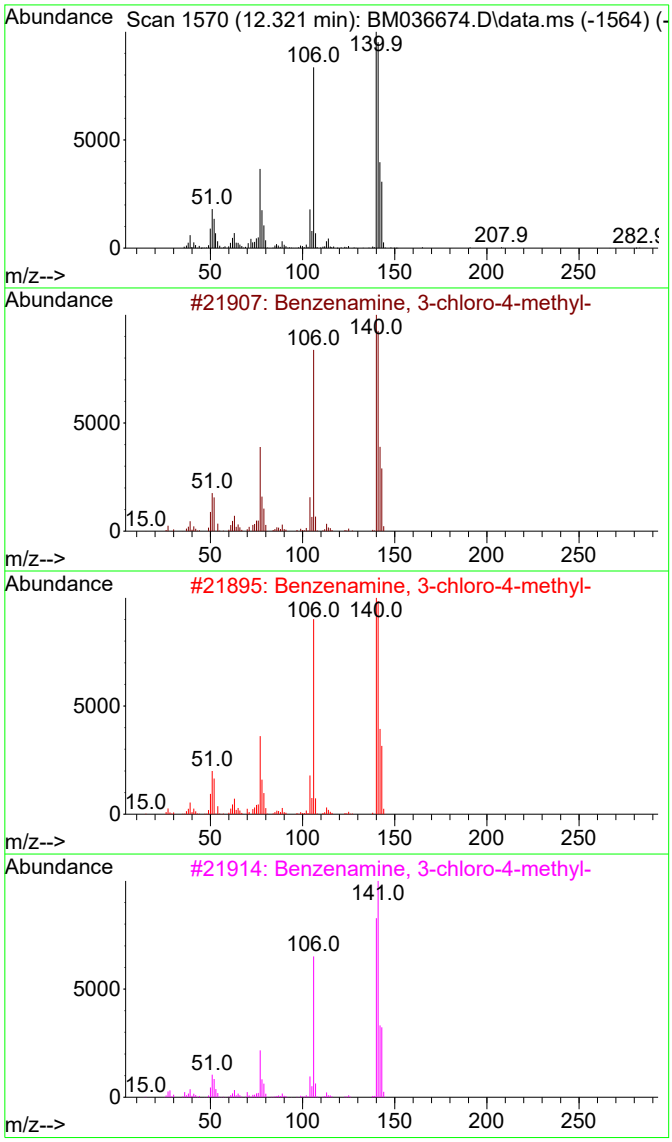
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM091522.M
Quant Title : SVOA CALIBRATION

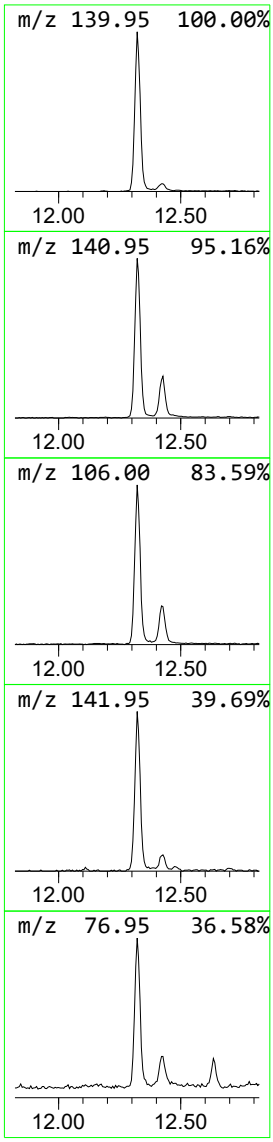
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzenamine, 3-chloro-4-met... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.321	3.01 ng/ul	670703	Naphthalene-d8	10.827

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 3-chloro-4-methyl-	141	C7H8ClN	000095-74-9	98
2	Benzenamine, 3-chloro-4-methyl-	141	C7H8ClN	000095-74-9	98
3	Benzenamine, 3-chloro-4-methyl-	141	C7H8ClN	000095-74-9	95
4	Benzenamine, 2-chloro-4-methyl-	141	C7H8ClN	000615-65-6	95
5	Benzenamine, 2-chloro-4-methyl-	141	C7H8ClN	000615-65-6	94





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Acq On : 23 Sep 2022 13:15
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Sample : N4595-06DL 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CB8H4DL

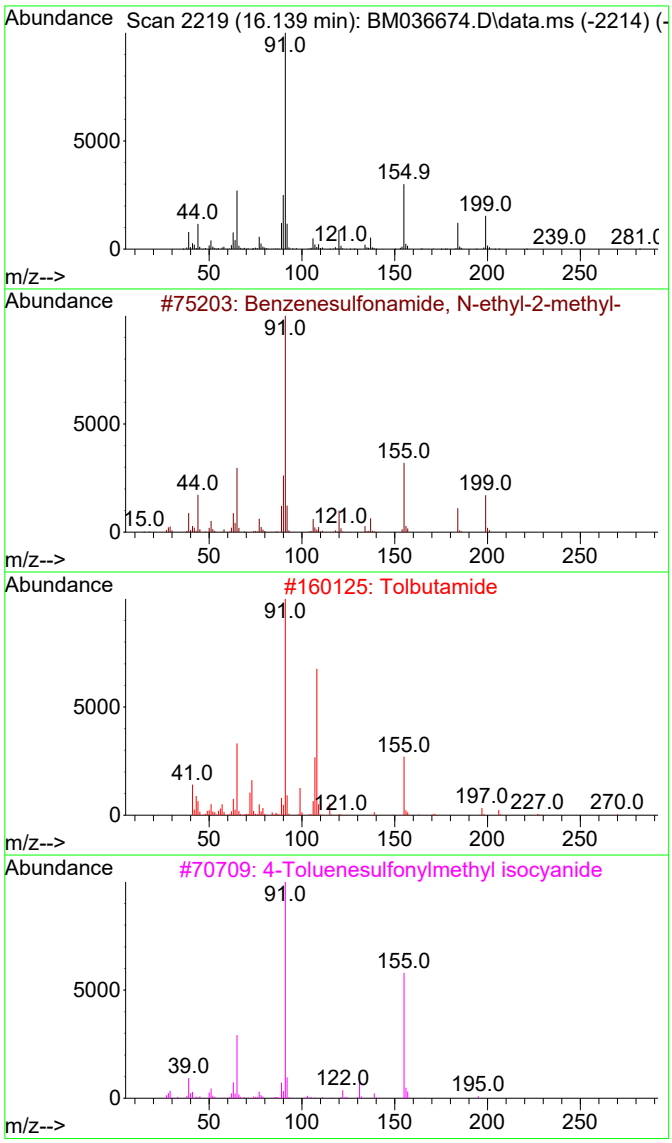
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM091522.M
Quant Title : SVOA CALIBRATION

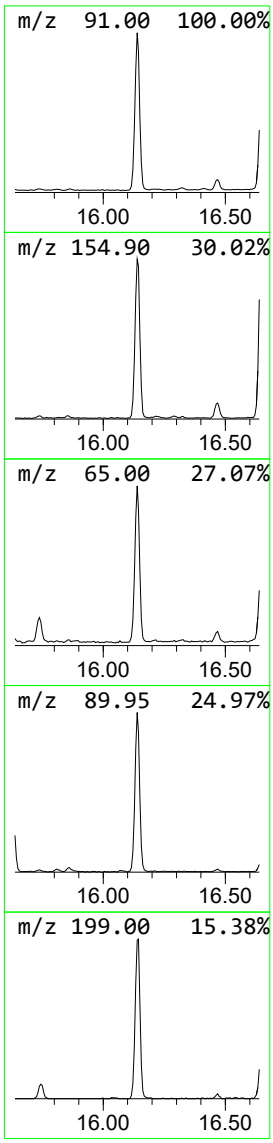
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzenesulfonamide, N-ethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.139	3.59 ng/ul	1152740	Phenanthrene-d10	17.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N-ethyl-2-me...	199	C9H13NO2S	001077-56-1	98
2	Tolbutamide	270	C12H18N2O3S	000064-77-7	50
3	4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	50
4	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	50
5	N3, N.alpha.-bis*ptoluenesulfony...	462	C20H22N4O5S2	1000130-21-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092322\
Data File : BM036674.D
Acq On : 23 Sep 2022 13:15
Operator : CG/JU
Sample : N4595-06DL 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CB8H4DL

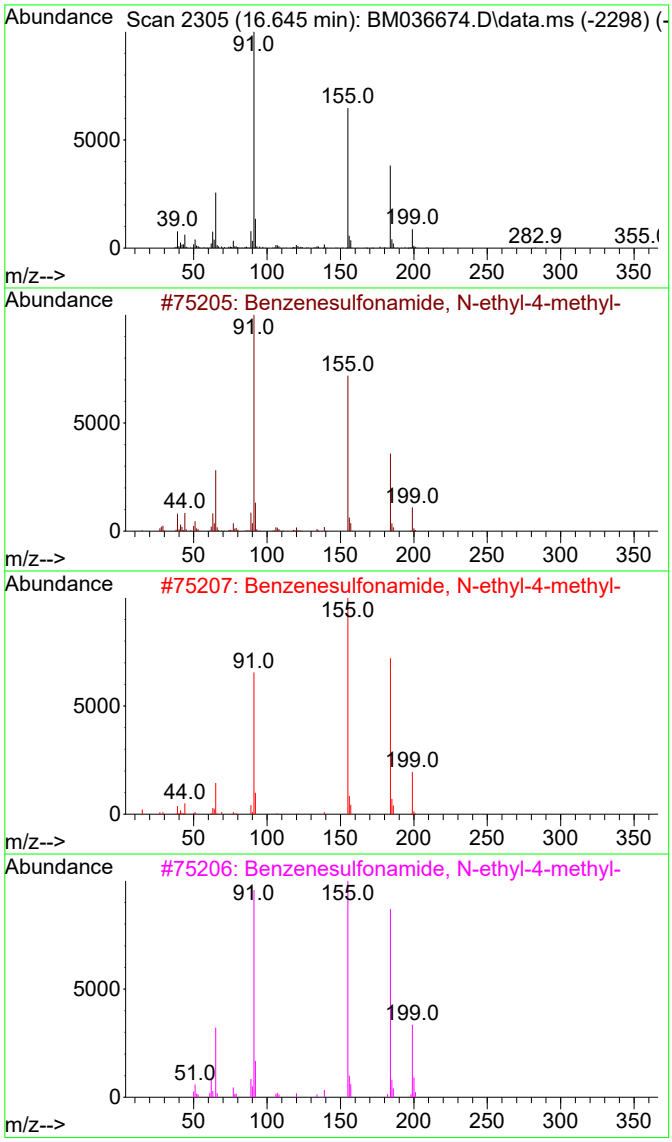
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM091522.M
Quant Title : SVOA CALIBRATION

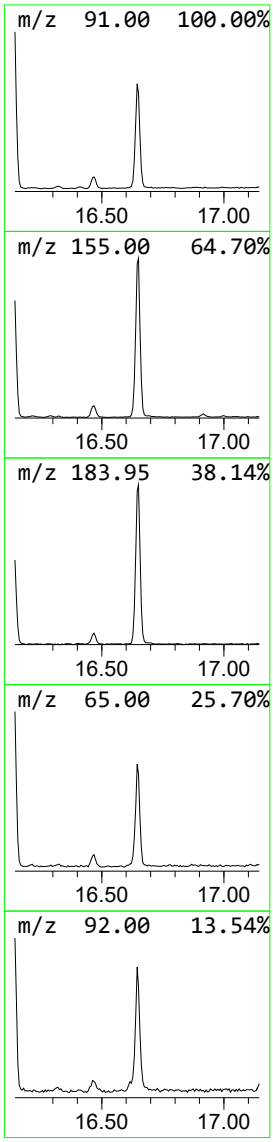
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzenesulfonamide, N-ethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.645	2.23 ng/ul	717122	Phenanthrene-d10	17.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	92
2	Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	91
3	Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	90
4	N-isobutyl-4-methylbenzenesulfon...	227	C11H17NO2S	023705-38-6	90
5	Furazan-3-carboxylic acid, 4-ami...	325	C12H15N5O4S	1000304-69-4	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092322\
Data File : BM036674.D
Acq On : 23 Sep 2022 13:15
Operator : CG/JU
Sample : N4595-06DL 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CB8H4DL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM091522.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
Butane, 2-metho...	3.122	39.9	ng/ul	5873970	1	8.016	2947380	20.0
Benzenamine, 3-...	9.004	9.3	ng/ul	1366600	1	8.016	2947380	20.0
Benzenamine, 3-...	12.321	3.0	ng/ul	670703	2	10.827	4461480	20.0
Benzenesulfonam...	16.139	3.6	ng/ul	1152740	4	17.380	6423560	20.0
Benzenesulfonam...	16.645	2.2	ng/ul	717122	4	17.380	6423560	20.0