LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018238.D
Acq On : 18 Nov 2023 01:21
Operator : MA/JU
Sample : 05369-22
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : GCDR7

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-BP111023.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP018238.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.158	9	12	21	rVB	16222	22286	1.00%	0.105%
2	3.599	84	87	100	rBV	78294	142895	6.43%	0.674%
3	3.776	114	117	120	rVB5	4306	4495	0.20%	0.021%
4	4.046	161	163	166	rVB4	2409	2377	0.11%	0.011%
5	4.411	222	225	229	rBV6	2492	3489	0.16%	0.016%
6	5.058	332	335	338	rBV5	1871	2754	0.12%	0.013%
7	6.687	607	612	630	rBV	212421	384543	17.31%	1.813%
8	6.811	630	633	635	rBV4	4396	5277	0.24%	0.025%
9	6.964	655	659	674	rVB2	41300	91632	4.12%	0.432%
10	7.128	682	687	699	rBV	235515	377892	17.01%	1.782%
11	7.305	711	717	729	rBV	231341	408845	18.40%	1.928%
12	7.781	792	798	811	rBV	212968	382404	17.21%	1.803%
13	8.140	854	859	861	rBV6	1896	3214	0.14%	0.015%
14	8.511	917	922	940	rBV	153461	319661	14.39%	1.507%
15	8.987	995	1003	1021	rBV	298103	562935	25.34%	2.654%
16	9.134	1024	1028	1029	rBV4	2251	2331	0.10%	0.011%
17	9.493	1086	1089	1094	rVB7	1583	2442	0.11%	0.012%
18	9.699	1117	1124	1138	rBV	252841	485839	21.87%	2.291%
19	9.963	1164	1169	1177	rVB4	8583	17901	0.81%	0.084%
20	10.228	1206	1214	1234	rBV	292666	641981	28.89%	3.027%
21	10.593	1268	1276	1292	rBV	302677	517264	23.28%	2.439%
22	10.775	1299	1307	1328	rBV	265871	611926	27.54%	2.885%
23	11.299	1389	1396	1408	rBV	115882	259364	11.67%	1.223%
24	11.428	1417	1418	1422	rVB4	3372	3163	0.14%	0.015%
25	11.652	1452	1456	1459	rVB3	4439	6517	0.29%	0.031%
26	11.775	1471	1477	1488	rVB	35193	56003	2.52%	0.264%
27	12.104	1527	1533	1548	rBV	60526	134626	6.06%	0.635%
28	12.216	1548	1552	1554	rVV5	3801	5166	0.23%	0.024%
29	12.234	1554	1555	1558	rVB3	4174	3139	0.14%	0.015%
30	12.722	1634	1638	1645	rBV7	3252	7228	0.33%	0.034%
31	13.028	1686	1690	1693	rVV6	1920	2228	0.10%	0.011%
32	13.304	1731	1737	1743	rVB10	4038	7167	0.32%	0.034%
33	13.422	1753	1757	1760	rVV5	1949	2798	0.13%	0.013%
34	13.451	1760	1762	1769	rVB8	1598	2313	0.10%	0.011%
35	13.669	1795	1799	1803	rBV7	2524	4391	0.20%	0.021%
36	13.757	1810	1814	1817	rBV5	5647	9759	0.44%	0.046%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018238.D
Acq On : 18 Nov 2023 01:21
Operator : MA/JU
Sample : 05369-22
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : GCDR7

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-BP111023.MA.M
Title : SVOA CALIBRATION

37	13.881	1826	1835	1847	rBV	821164	1178320	53.03%	5.556%
38	13.957	1847	1848	1852	rVB4	3367	2786	0.13%	0.013%
39	14.081	1866	1869	1872	rVB5	1842	2301	0.10%	0.011%
40	14.157	1876	1882	1892	rVV	851405	1215129	54.69%	5.729%
41	14.234	1892	1895	1898	rVB5	2252	3740	0.17%	0.018%
42	14.422	1922	1927	1930	rBV	557767	729290	32.82%	3.438%
43	14.457	1930	1933	1947	rVB	480617	707532	31.84%	3.336%
44	14.687	1967	1972	1981	rBV	2754	7138	0.32%	0.034%
45	14.798	1985	1991	1994	rBV5	12510	23411	1.05%	0.110%
46	15.251	2065	2068	2070	rVB4	2879	2889	0.13%	0.014%
47	15.463	2098	2104	2119	rBV	1170536	1697179	76.39%	8.002%
48	15.622	2125	2131	2143	rBV	317011	553738	24.92%	2.611%
49	15.716	2143	2147	2153	rVB6	17272	30931	1.39%	0.146%
50	16.245	2231	2237	2255	rBV3	50784	164328	7.40%	0.775%
51	17.057	2370	2375	2376	rBV5	1873	2456	0.11%	0.012%
52	17.240	2400	2406	2414	rBV	661123	919312	41.38%	4.334%
53	17.340	2417	2423	2440	rVV2	1281568	1860545	83.74%	8.772%
54	17.504	2449	2451	2457	rVB7	2330	3175	0.14%	0.015%
55	17.987	2529	2533	2537	rBV5	4383	6600	0.30%	0.031%
56	18.051	2540	2544	2548	rBV6	5340	6812	0.31%	0.032%
57	18.098	2548	2552	2563	rVV6	10612	26512	1.19%	0.125%
58	18.375	2596	2599	2604	rVB6	4583	5653	0.25%	0.027%
59	18.592	2632	2636	2641	rVB7	7255	9040	0.41%	0.043%
60	18.945	2692	2696	2698	rBV5	3707	4235	0.19%	0.020%
61	19.175	2731	2735	2739	rBV3	15842	22504	1.01%	0.106%
62	19.251	2745	2748	2753	rVB3	12069	15736	0.71%	0.074%
63	19.345	2760	2764	2767	rBV5	9793	16008	0.72%	0.075%
64	19.598	2801	2807	2823	rBV	1732980	2221849	100.00%	10.476%
65	21.375	3104	3109	3120	rBV	741280	1017653	45.80%	4.798%
66	23.680	3494	3501	3514	rVB2	1138492	2221020	99.96%	10.472%
67	23.845	3523	3529	3542	rVB	479787	1033510	46.52%	4.873%

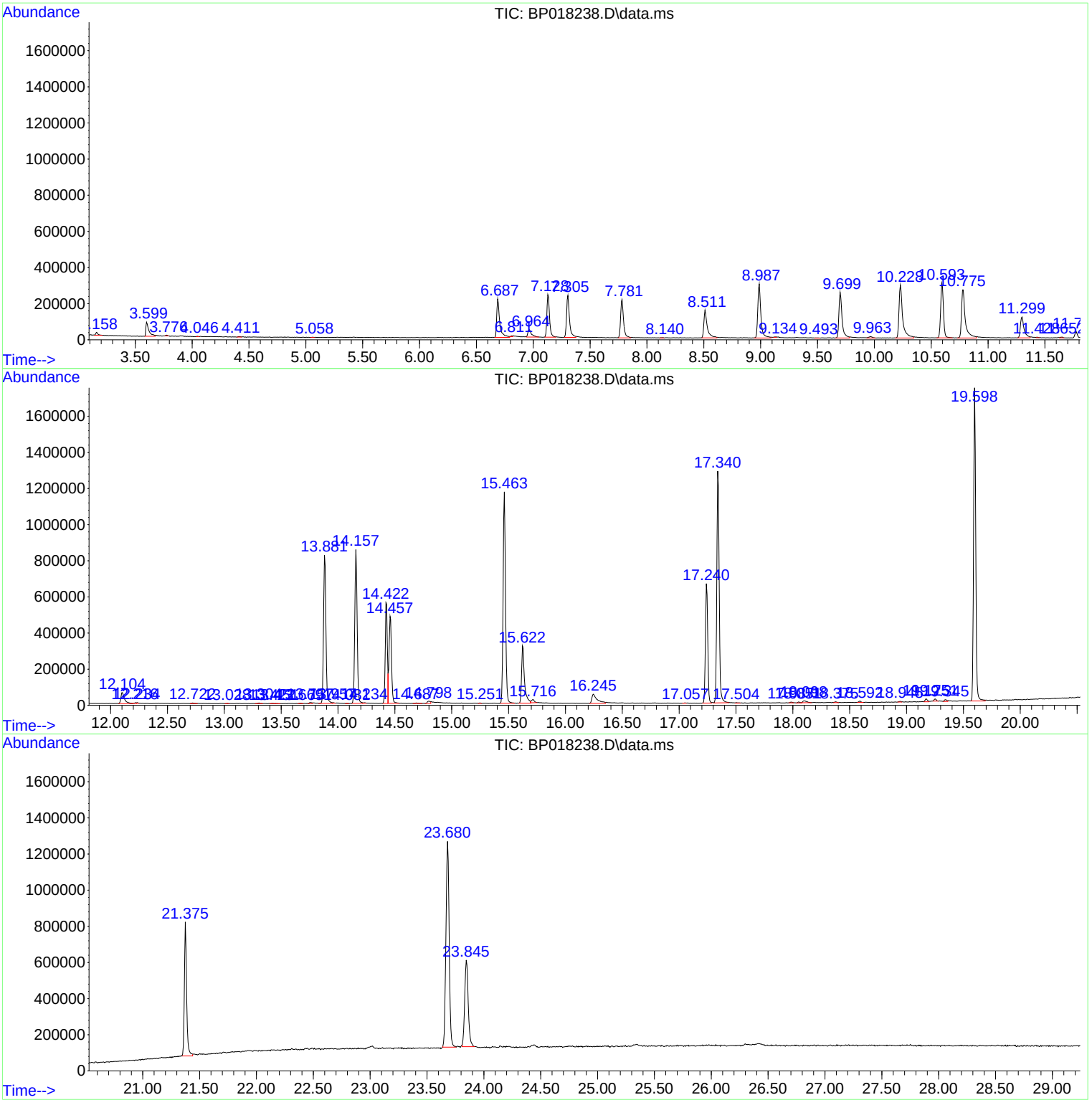
Sum of corrected areas: 21209577

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018238.D
Acq On : 18 Nov 2023 01:21
Operator : MA/JU
Sample : 05369-22
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDR7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.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\BP111723\
Data File : BP018238.D
Acq On : 18 Nov 2023 01:21
Operator : MA/JU
Sample : 05369-22
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Instrument :
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ClientSampleId :
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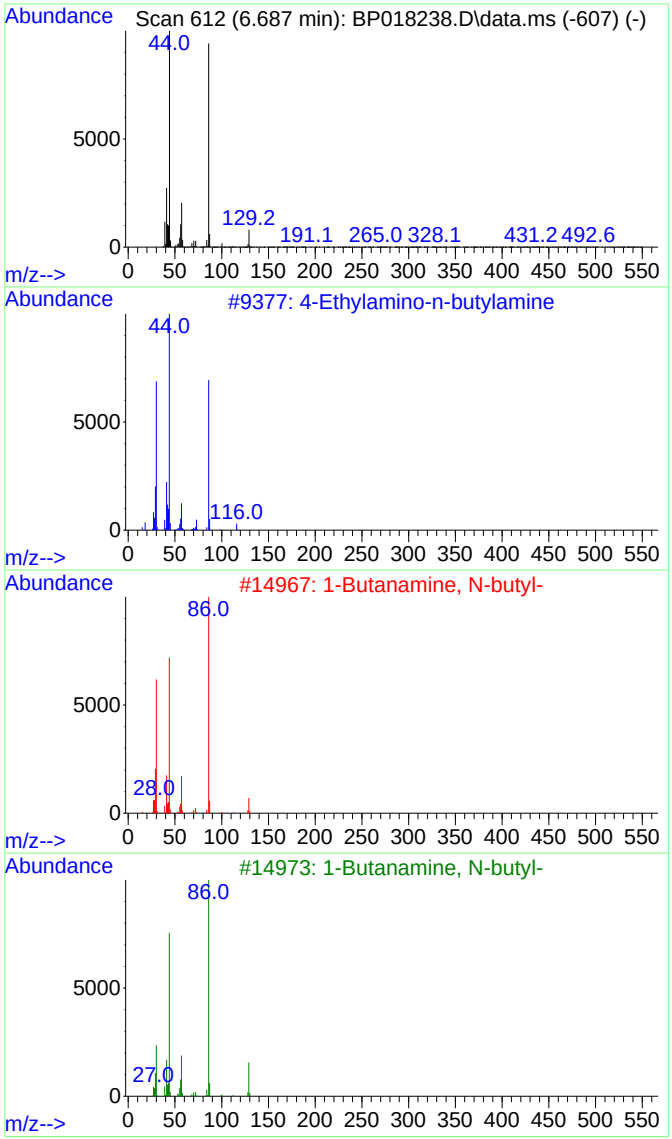
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

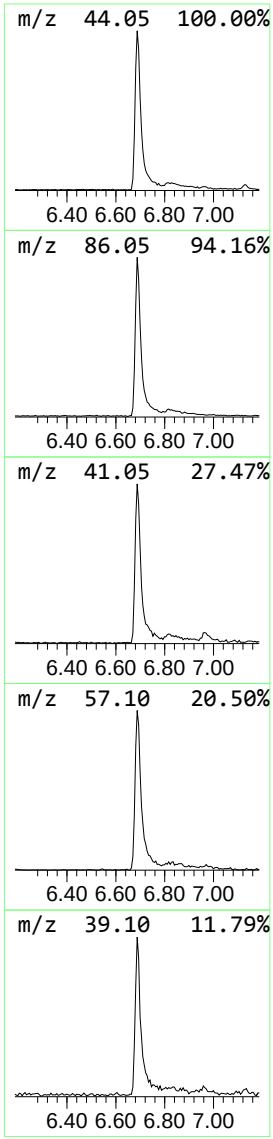
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 4-Ethylamino-n-butylamine Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.687	20.11 ng/ul	384543	1,4-Dichlorobenzene-d4	7.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Ethylamino-n-butylamine	116	C6H16N2	064429-16-9	90
2	1-Butanamine, N-butyl-	129	C8H19N	000111-92-2	86
3	1-Butanamine, N-butyl-	129	C8H19N	000111-92-2	83
4	n-Butylethylenediamine	116	C6H16N2	019522-69-1	78
5	N-sec-Butyl-n-propylamine	115	C7H17N	039190-67-5	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018238.D
Acq On : 18 Nov 2023 01:21
Operator : MA/JU
Sample : 05369-22
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDR7

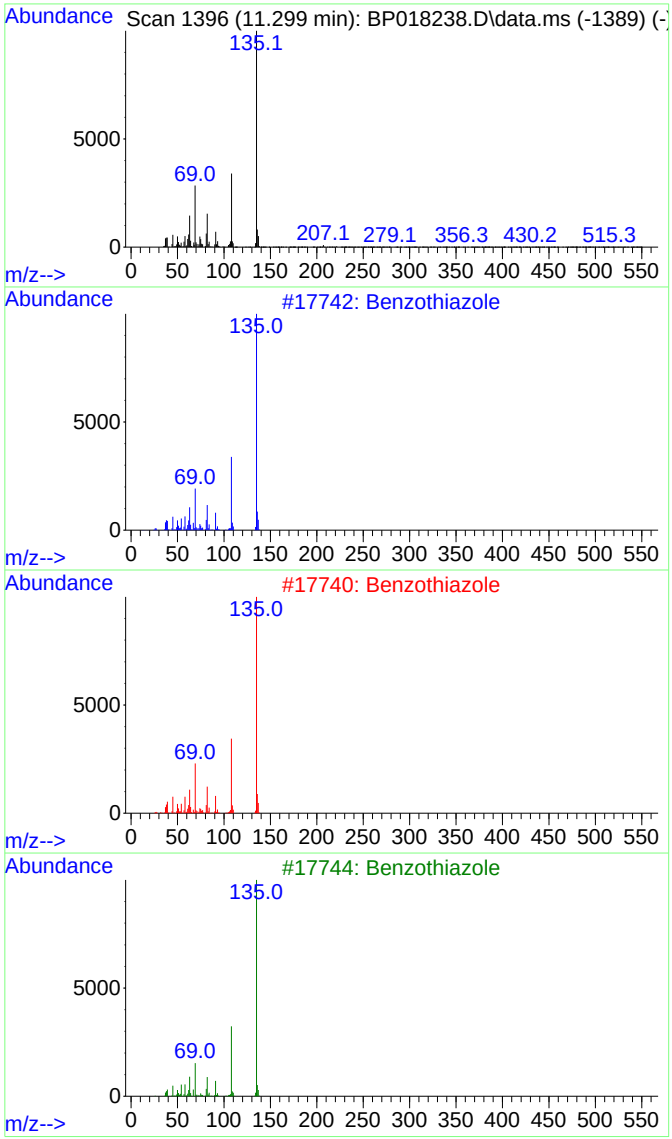
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

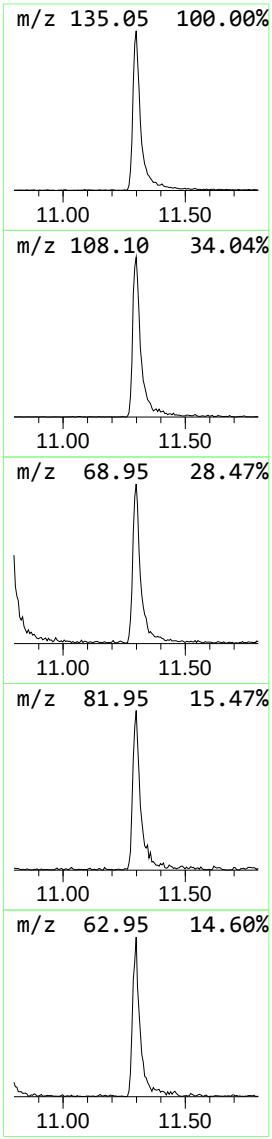
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzothiazole Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.299	10.03 ng/ul	259364	Naphthalene-d8	10.593

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	95
2	Benzothiazole	135	C7H5NS	000095-16-9	93
3	Benzothiazole	135	C7H5NS	000095-16-9	91
4	Benzothiazole	135	C7H5NS	000095-16-9	90
5	Benzothiazole	135	C7H5NS	000095-16-9	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018238.D
Acq On : 18 Nov 2023 01:21
Operator : MA/JU
Sample : 05369-22
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDR7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

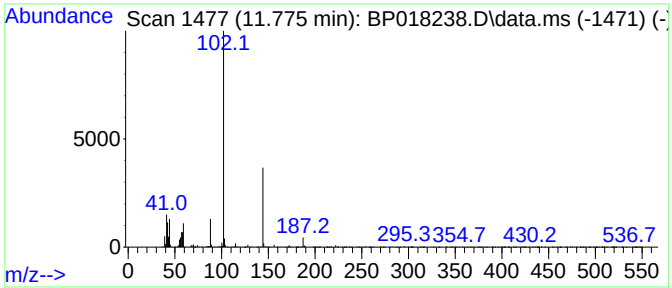
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

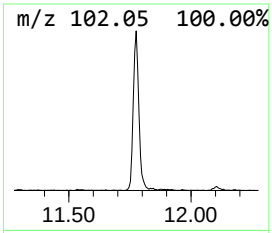
****

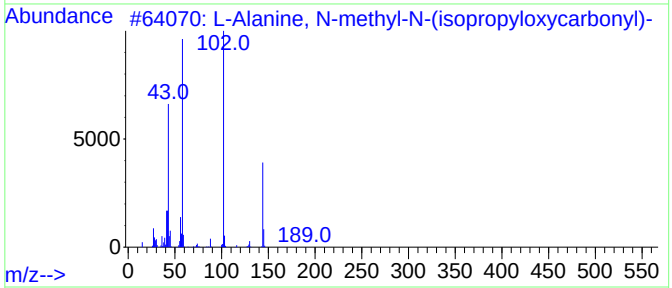
Peak Number 3 unknown-01 Concentration Rank 5

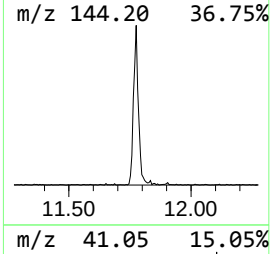
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.775	2.17 ng/ul	56003	Naphthalene-d8	10.593

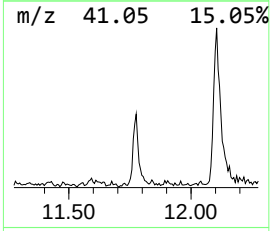
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	L-Alanine, N-methyl-N-(isopropyl...	189	C8H15NO4	1000454-81-2	39
2	1-N-(tert-Butyl-oxo-azanylidene)...	203	C6H13N5O3	1000443-73-2	38
3	l-Alanyl-l-isoleucine, N-methoxy...	342	C13H21F3N2O5	1000322-59-8	38
4	Ala-Ala, N-methoxycarbonyl-, met...	232	C9H16N2O5	1010467-85-5	38
5	l-Alanine, N-methoxycarbonyl-, h...	371	C21H41NO4	1000313-38-4	37

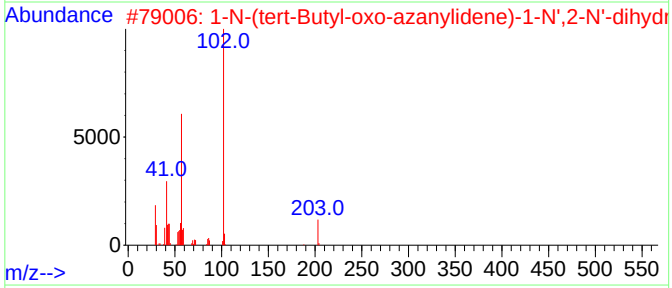


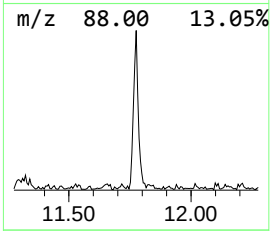


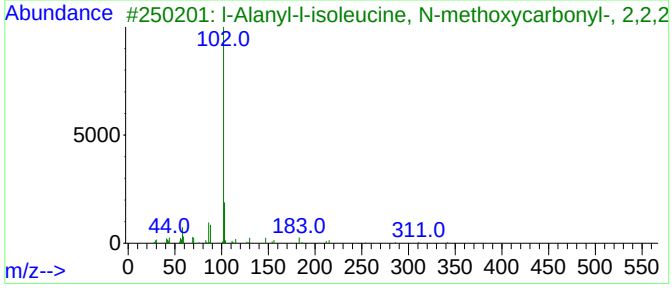


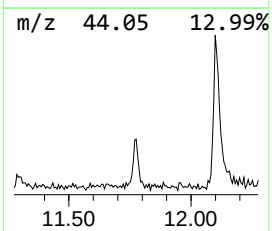












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018238.D
Acq On : 18 Nov 2023 01:21
Operator : MA/JU
Sample : 05369-22
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDR7

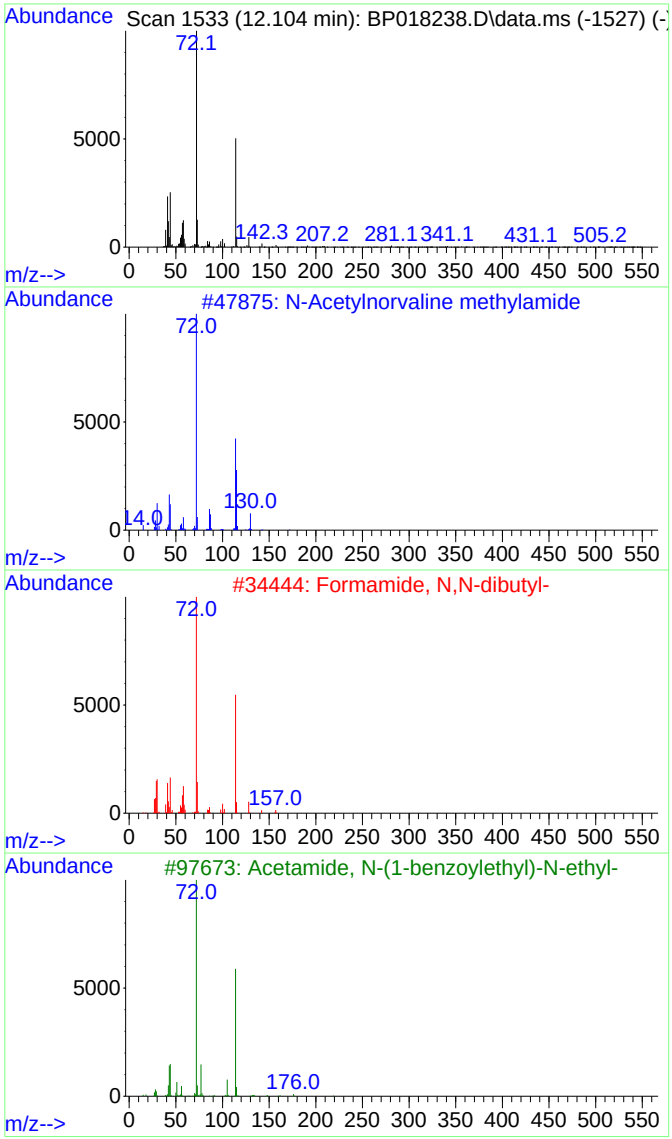
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

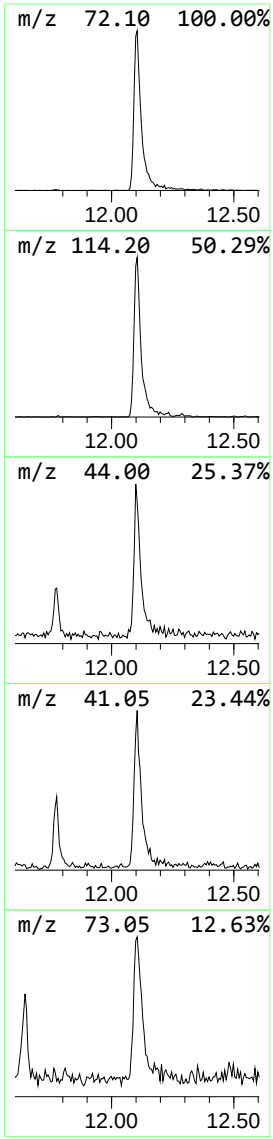
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 N-Acetylnorvaline methylamide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.105	5.21 ng/ul	134626	Naphthalene-d8	10.593

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Acetylnorvaline methylamide	172	C8H16N2O2	033067-46-8	64
2	Formamide, N,N-dibutyl-	157	C9H19NO	000761-65-9	64
3	Acetamide, N-(1-benzoylethyl)-N-...	219	C13H17NO2	055116-37-5	59
4	4-Methylethcathinone, N-acetyl-	233	C14H19NO2	1000448-37-4	59
5	Butylone, N-acetyl-	263	C14H17NO4	1000448-48-2	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018238.D
Acq On : 18 Nov 2023 01:21
Operator : MA/JU
Sample : 05369-22
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDR7

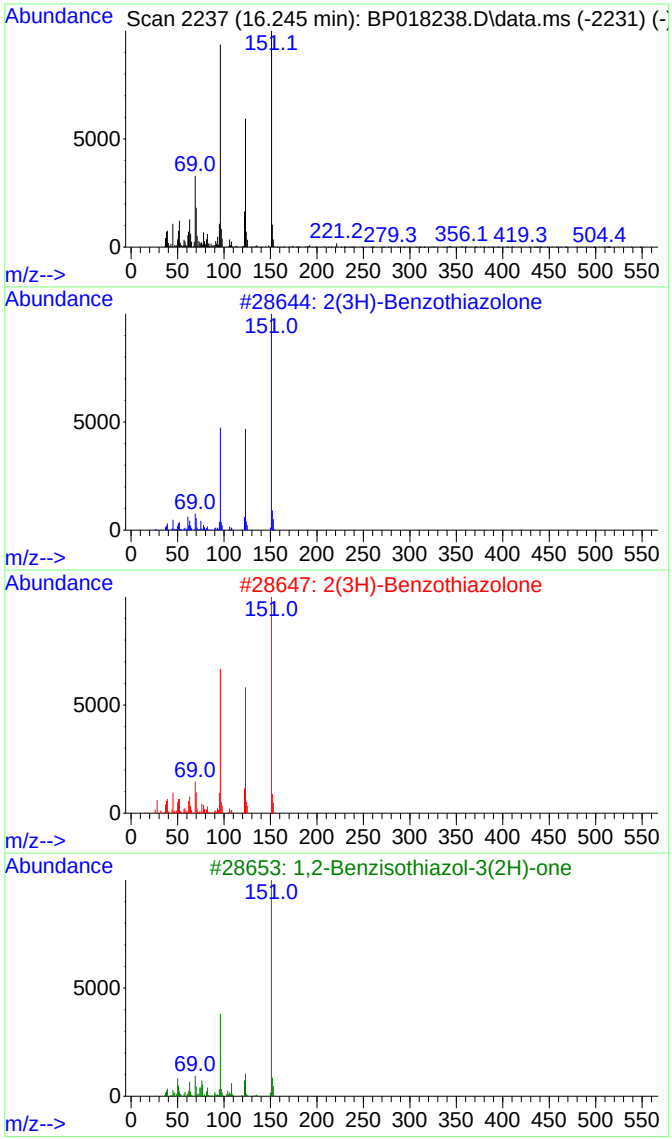
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

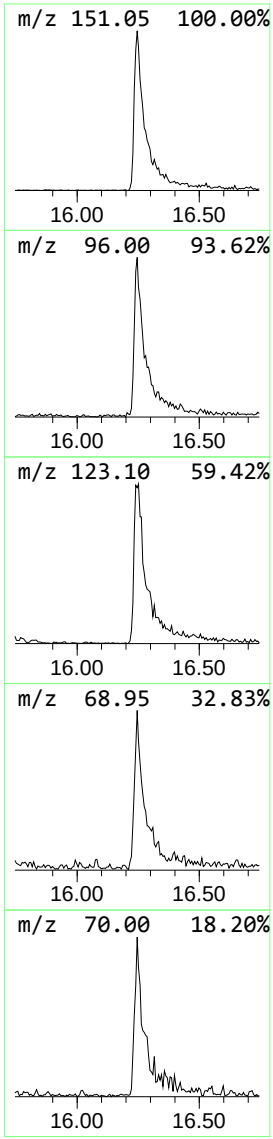
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2(3H)-Benzothiazolone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.245	3.58 ng/ul	164328	Phenanthrene-d10	17.240

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	91
2	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	81
3	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	59
4	4-Methoxyformanilide	151	C8H9NO2	005470-34-8	38
5	RCH 108	151	C7H5NO3	002297-94-1	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018238.D
Acq On : 18 Nov 2023 01:21
Operator : MA/JU
Sample : 05369-22
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDR7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.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
4-Ethylamino-n-...	6.687	20.1	ng/ul	384543	1	7.781	382404	20.0
Benzothiazole	11.299	10.0	ng/ul	259364	2	10.593	517264	20.0
unknown-01	11.775	2.2	ng/ul	56003	2	10.593	517264	20.0
N-Acetylnorvali...	12.105	5.2	ng/ul	134626	2	10.593	517264	20.0
2(3H)-Benzothia...	16.245	3.6	ng/ul	164328	4	17.240	919312	20.0