LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081221\
Data File : BG049817.D
Acq On : 12 Aug 2021 14:22
Operator : CG/JU
Sample : M3333-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 124042

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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_G\Methods\8270-BG080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049817.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.131	12	16	21	rBV2	66892	99468	5.23%	0.710%
2	3.184	21	25	31	rVB6	11142	21201	1.12%	0.151%
3	5.105	347	352	360	rVB	24290	43003	2.26%	0.307%
4	5.587	427	434	446	rBV	457258	760908	40.04%	5.431%
5	7.196	693	708	718	rBV	498567	896300	47.17%	6.398%
6	8.030	844	850	857	rVB2	103298	175958	9.26%	1.256%
7	9.205	1040	1050	1058	rBV	306292	563161	29.64%	4.020%
8	10.615	1284	1290	1301	rBV5	33643	69071	3.63%	0.493%
9	10.856	1323	1331	1339	rBV	153127	285520	15.03%	2.038%
10	13.306	1739	1748	1755	rBV	886023	1366287	71.90%	9.753%
11	13.570	1787	1793	1798	rBV2	19219	28719	1.51%	0.205%
12	14.686	1977	1983	1990	rBV	280316	439634	23.14%	3.138%
13	16.178	2230	2237	2249	rBV	823367	1267322	66.69%	9.046%
14	17.441	2443	2452	2456	rBV	328644	520946	27.41%	3.719%
15	17.482	2456	2459	2464	rVB	64915	86175	4.53%	0.615%
16	17.570	2470	2474	2479	rVB3	17794	27198	1.43%	0.194%
17	18.316	2594	2601	2605	rBV3	21196	32008	1.68%	0.228%
18	18.363	2605	2609	2617	rVB4	15149	24532	1.29%	0.175%
19	18.510	2628	2634	2639	rBV2	24463	49344	2.60%	0.352%
20	18.857	2688	2693	2697	rVB5	15582	22183	1.17%	0.158%
21	19.227	2753	2756	2758	rBV4	15536	19318	1.02%	0.138%
22	19.256	2758	2761	2765	rVB4	39796	47118	2.48%	0.336%
23	19.374	2775	2781	2783	rBV2	21597	36510	1.92%	0.261%
24	19.491	2795	2801	2807	rBV	333452	474147	24.95%	3.384%
25	19.732	2838	2842	2848	rBV2	20625	34970	1.84%	0.250%
26	19.826	2852	2858	2859	rBV2	54949	79348	4.18%	0.566%
27	19.856	2859	2863	2870	rVB	319382	465492	24.50%	3.323%
28	20.049	2889	2896	2901	rBV	1441065	1900260	100.00%	13.564%
29	20.179	2912	2918	2924	rBV3	22678	51274	2.70%	0.366%
30	20.349	2934	2947	2951	rBV	50506	131312	6.91%	0.937%
31	20.449	2959	2964	2967	rBV	30841	45376	2.39%	0.324%
32	20.508	2967	2974	2977	rVV3	21446	41778	2.20%	0.298%
33	20.643	2994	2997	3001	rBV4	16547	22766	1.20%	0.163%
34	20.684	3001	3004	3008	rBV6	20158	29985	1.58%	0.214%
35	21.113	3073	3077	3083	rVB3	26922	45836	2.41%	0.327%
36	21.301	3102	3109	3112	rBV4	39050	73946	3.89%	0.528%

LSC Area Percent Report

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Sample : M3333-11
Misc :
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Instrument : BNA_G
ClientSampleId : 124042

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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_G\Methods\8270-BG080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.348	3112	3117	3121	rBV4	45242	81440	4.29%	0.581%
38	21.442	3129	3133	3139	rVB2	37472	72114	3.79%	0.515%
39	21.718	3172	3180	3186	rBV2	324791	827662	43.56%	5.908%
40	21.771	3186	3189	3196	rVB	151037	231971	12.21%	1.656%
41	21.923	3211	3215	3222	rVB2	49032	85624	4.51%	0.611%
42	21.994	3223	3227	3232	rVB7	13355	26040	1.37%	0.186%
43	22.129	3246	3250	3258	rBV3	24061	50572	2.66%	0.361%
44	23.962	3553	3562	3569	rBV2	173503	567294	29.85%	4.049%
45	24.226	3601	3607	3612	rVB2	31790	73660	3.88%	0.526%
46	24.696	3679	3687	3699	rVB	110995	325954	17.15%	2.327%
47	24.843	3704	3712	3726	rVB	150137	437184	23.01%	3.121%
48	25.002	3729	3739	3747	rBV3	170121	522160	27.48%	3.727%
49	28.749	4365	4377	4388	rBV3	71626	323985	17.05%	2.313%
50	29.913	4566	4575	4576	rBV9	52067	105349	5.54%	0.752%

Sum of corrected areas: 14009383

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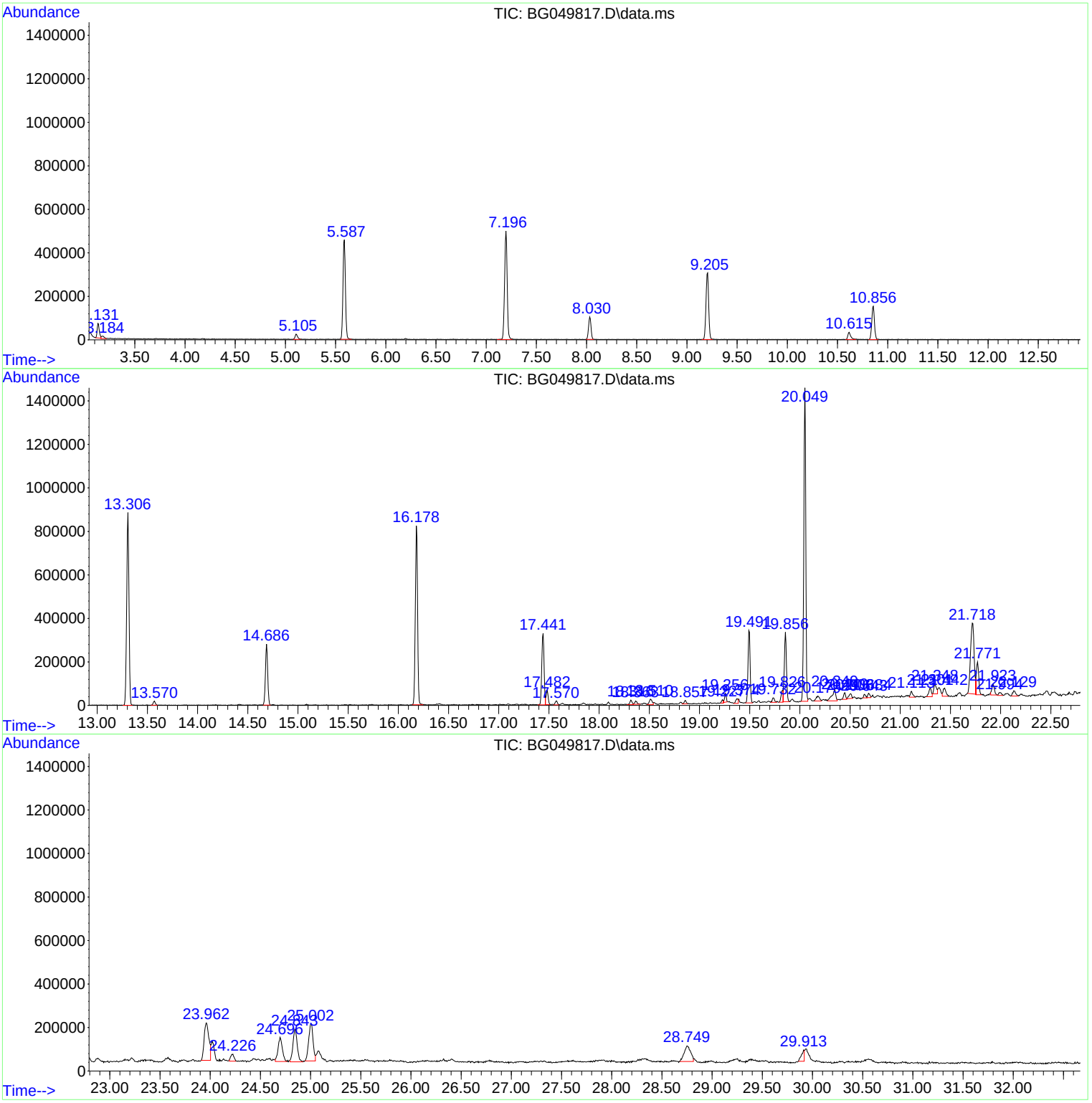
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
124042

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081221\
Data File : BG049817.D
Acq On : 12 Aug 2021 14:22
Operator : CG/JU
Sample : M3333-11
Misc :
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Instrument : BNA_G
ClientSampleId : 124042

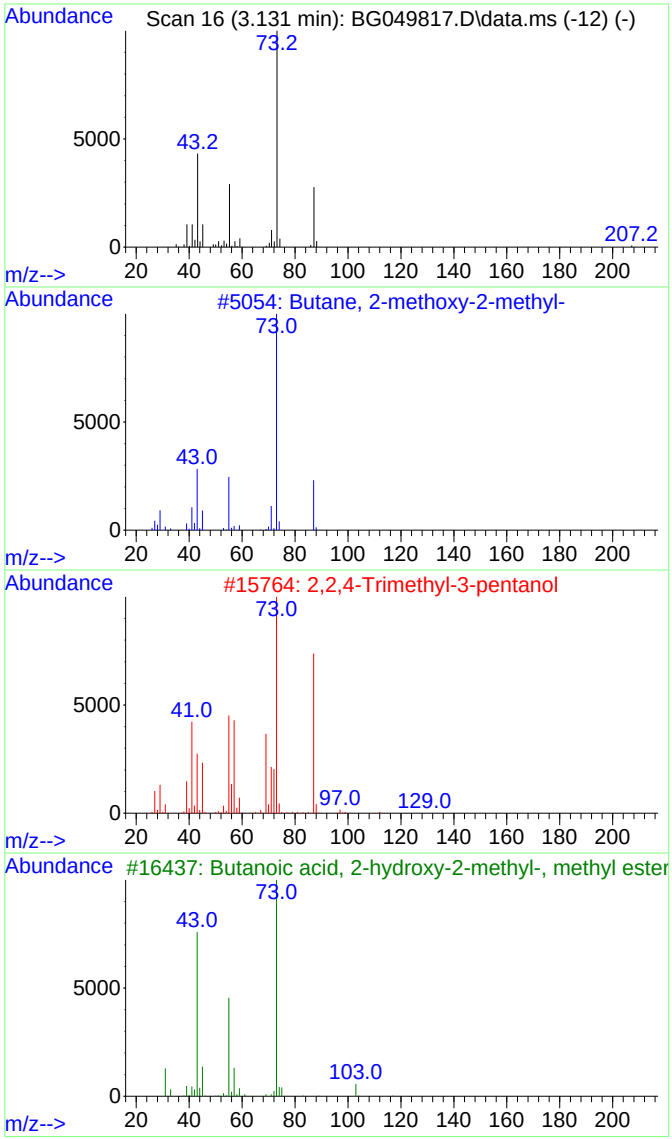
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

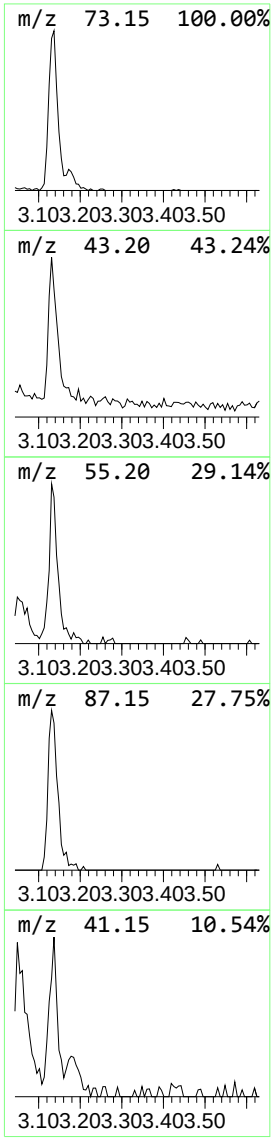
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.131	11.31 ng	99468	1,4-Dichlorobenzene-d4	8.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	50
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	37
4	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
5	3-Pentanol, 2,3-dimethyl-	116	C7H16O	000595-41-5	36





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Operator : CG/JU
Sample : M3333-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 124042

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

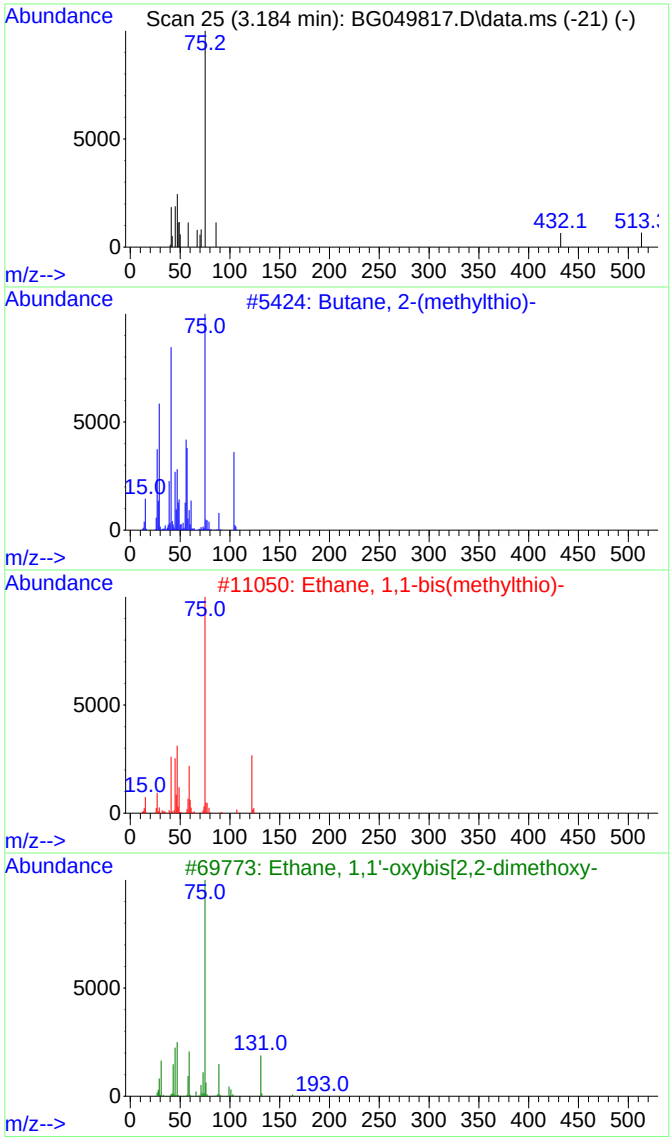
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

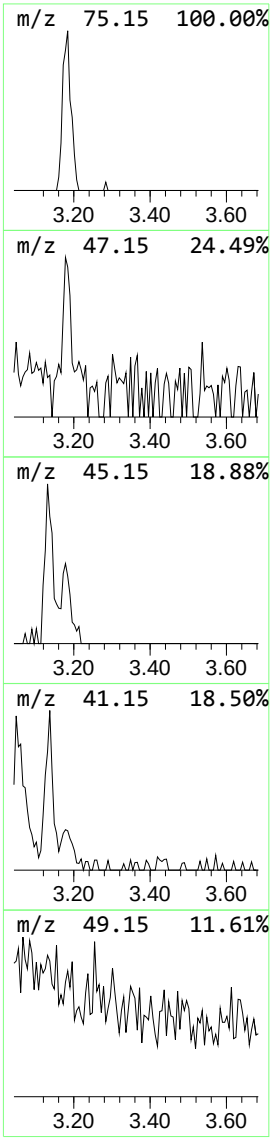
****

Peak Number 2 Butane, 2-(methylthio)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.184	2.41 ng	21201	1,4-Dichlorobenzene-d4	8.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-(methylthio)-	104	C5H12S	010359-64-5	59
2	Ethane, 1,1-bis(methylthio)-	122	C4H10S2	007379-30-8	38
3	Ethane, 1,1'-oxybis[2,2-dimethoxy-	194	C8H18O5	078082-46-9	9
4	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	9
5	4-Aminobutyraldehyde diethyl acetal	161	C8H19NO2	006346-09-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081221\
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Operator : CG/JU
Sample : M3333-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 124042

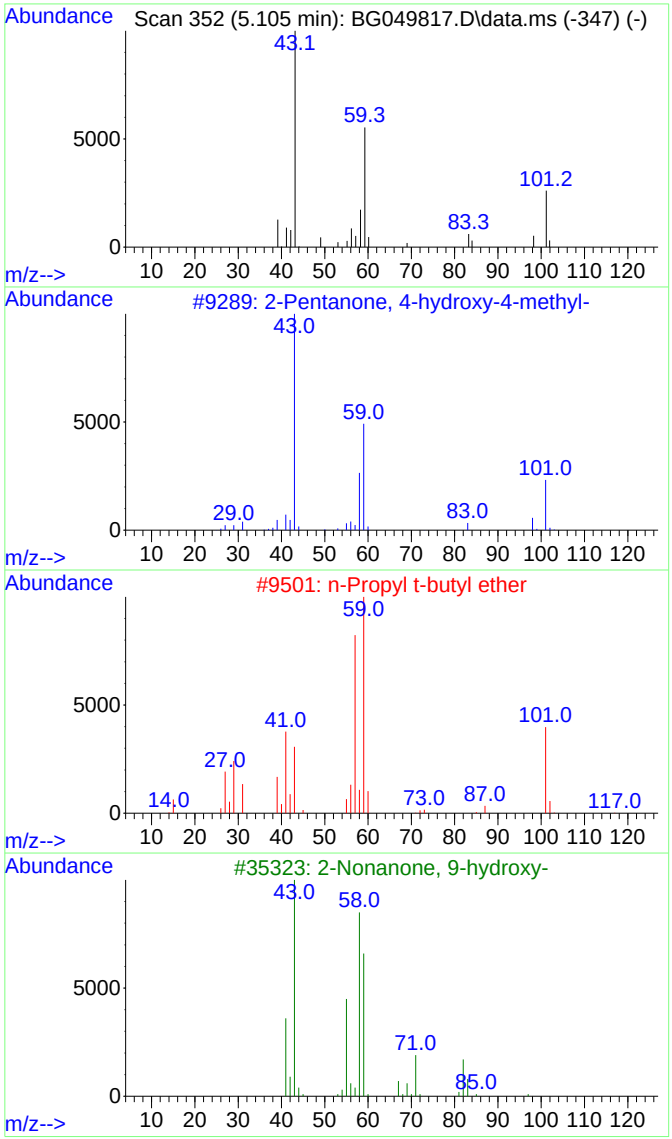
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

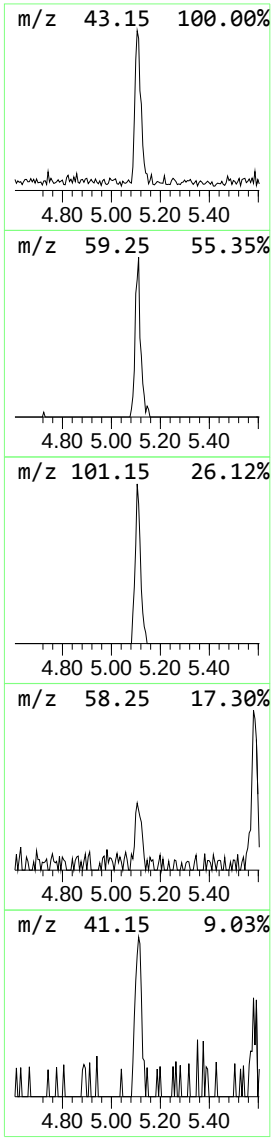
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.105	4.89 ng	43003	1,4-Dichlorobenzene-d4	8.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	38
3	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	25
4	3-Octanol	130	C8H18O	000589-98-0	10
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Acq On : 12 Aug 2021 14:22
Operator : CG/JU
Sample : M3333-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 124042

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

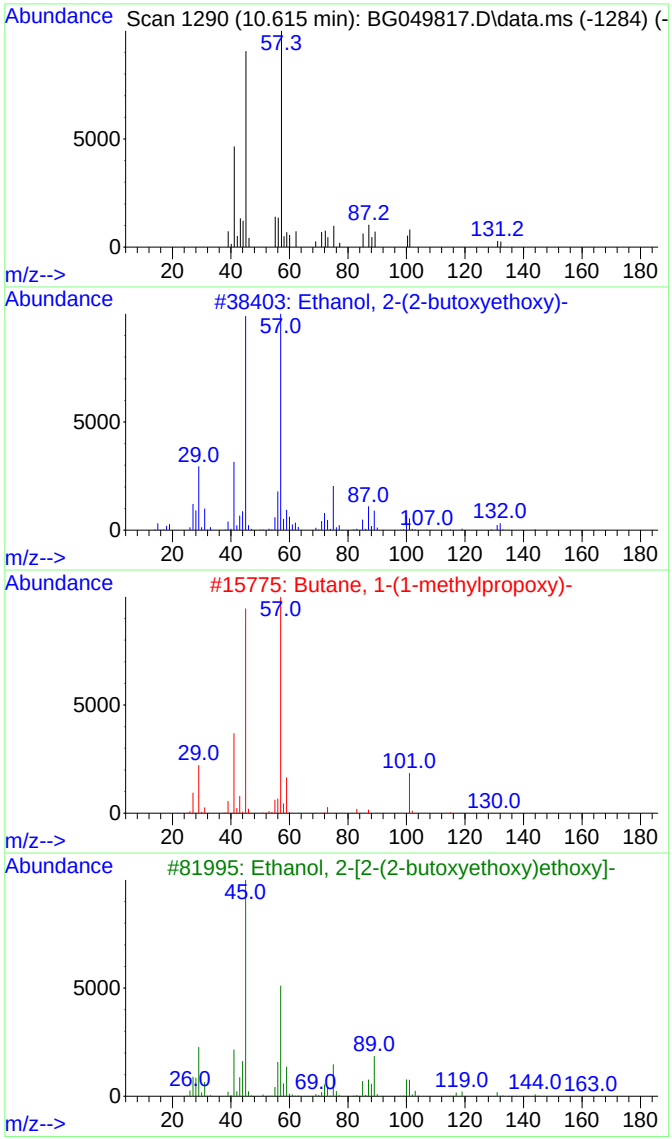
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

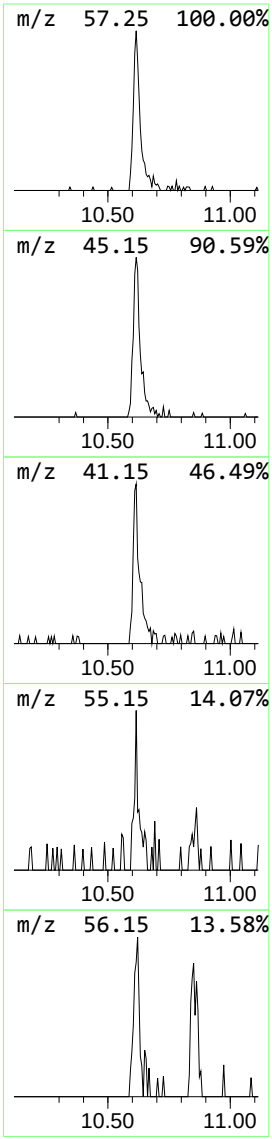
****

Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.615	4.84 ng	69071	Naphthalene-d8	10.856

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	59
3	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	56
4	DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	53
5	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	47





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Sample : M3333-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 124042

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

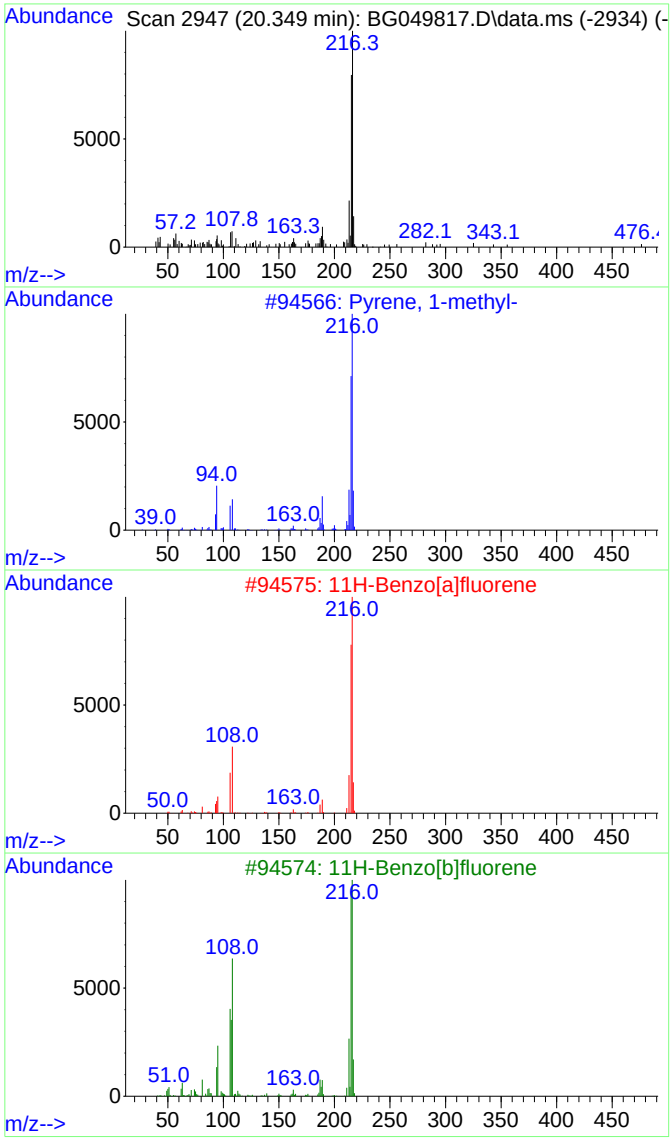
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

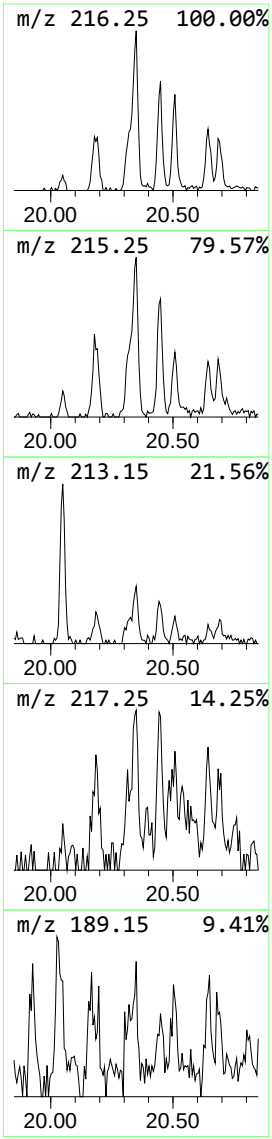
****

Peak Number 5 Pyrene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.349	3.17 ng	131312	Chrysene-d12	21.724

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081221\
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Quant Title : ASP BNA STANDARDS FOR 5 POINT 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...	3.131	11.3	ng	99468	1	8.030	175958	20.0
Butane, 2-(meth...	3.184	2.4	ng	21201	1	8.030	175958	20.0
2-Pentanone, 4-...	5.105	4.9	ng	43003	1	8.030	175958	20.0
Ethanol, 2-(2-b...	10.615	4.8	ng	69071	2	10.856	285520	20.0
Pyrene, 1-methyl-	20.349	3.2	ng	131312	5	21.724	827662	20.0