LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048952.D
Acq On : 14 Jun 2021 16:47
Operator : CG/JU
Sample : M2687-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DUP-01

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-BG061121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048952.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.170	16	22	33	rVB	153684	266176	23.00%	2.990%
2	3.293	37	43	50	rVB	55153	84374	7.29%	0.948%
3	4.274	205	210	217	rVB5	9547	19025	1.64%	0.214%
4	4.827	299	304	310	rBV4	7636	13430	1.16%	0.151%
5	5.197	363	367	377	rBV2	36047	62471	5.40%	0.702%
6	5.661	440	446	455	rVV	400948	682131	58.95%	7.661%
7	5.737	455	459	468	rVB2	17217	37811	3.27%	0.425%
8	6.119	518	524	527	rBV4	8222	14390	1.24%	0.162%
9	6.295	548	554	561	rVB5	5757	12653	1.09%	0.142%
10	7.259	709	718	727	rBV	423480	747496	64.60%	8.395%
11	8.117	857	864	871	rBV	133369	236068	20.40%	2.651%
12	9.286	1055	1063	1072	rBV	245814	451612	39.03%	5.072%
13	10.702	1297	1304	1314	rBV	157258	282691	24.43%	3.175%
14	10.943	1338	1345	1353	rVB	179145	324988	28.09%	3.650%
15	13.381	1754	1760	1769	rBV	527931	848120	73.30%	9.526%
16	14.762	1989	1995	2002	rBV	289050	469168	40.55%	5.269%
17	16.160	2228	2233	2239	rBV	38681	54612	4.72%	0.613%
18	16.243	2241	2247	2260	rVB	474230	763139	65.95%	8.571%
19	17.512	2456	2463	2469	rBV	386314	587099	50.74%	6.594%
20	17.623	2476	2482	2487	rVB5	37502	59357	5.13%	0.667%
21	18.176	2570	2576	2580	rBV3	36151	56118	4.85%	0.630%
22	18.393	2609	2613	2618	rBV4	38700	53710	4.64%	0.603%
23	18.693	2660	2664	2671	rBV9	9803	14471	1.25%	0.163%
24	19.339	2767	2774	2778	rBV8	26615	48917	4.23%	0.549%
25	19.545	2803	2809	2813	rBV9	7026	15182	1.31%	0.171%
26	19.662	2825	2829	2836	rVB7	22014	36500	3.15%	0.410%
27	19.897	2866	2869	2872	rVB5	11635	13785	1.19%	0.155%
28	20.115	2900	2906	2912	rBV	877966	1157128	100.00%	12.996%
29	20.420	2955	2958	2963	rVB7	7830	12554	1.08%	0.141%
30	20.596	2983	2988	2995	rBV7	6380	17483	1.51%	0.196%
31	20.878	3032	3036	3040	rVB5	18948	26909	2.33%	0.302%
32	21.442	3127	3132	3139	rBV5	35485	65644	5.67%	0.737%
33	21.689	3170	3174	3182	rVB2	35881	63004	5.44%	0.708%
34	21.801	3187	3193	3203	rVB2	363939	639998	55.31%	7.188%
35	22.647	3335	3337	3342	rBV5	7979	12413	1.07%	0.139%
36	23.029	3398	3402	3408	rVB8	19479	35700	3.09%	0.401%

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
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Misc :
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Instrument : BNA_G
ClientSampleId : DUP-01

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-BG061121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.575	3493	3495	3500	rVB6	11677	12280	1.06%	0.138%
38	25.138	3752	3761	3771	rVB	207685	604986	52.28%	6.795%

Sum of corrected areas: 8903593

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Instrument :
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ClientSampleId :
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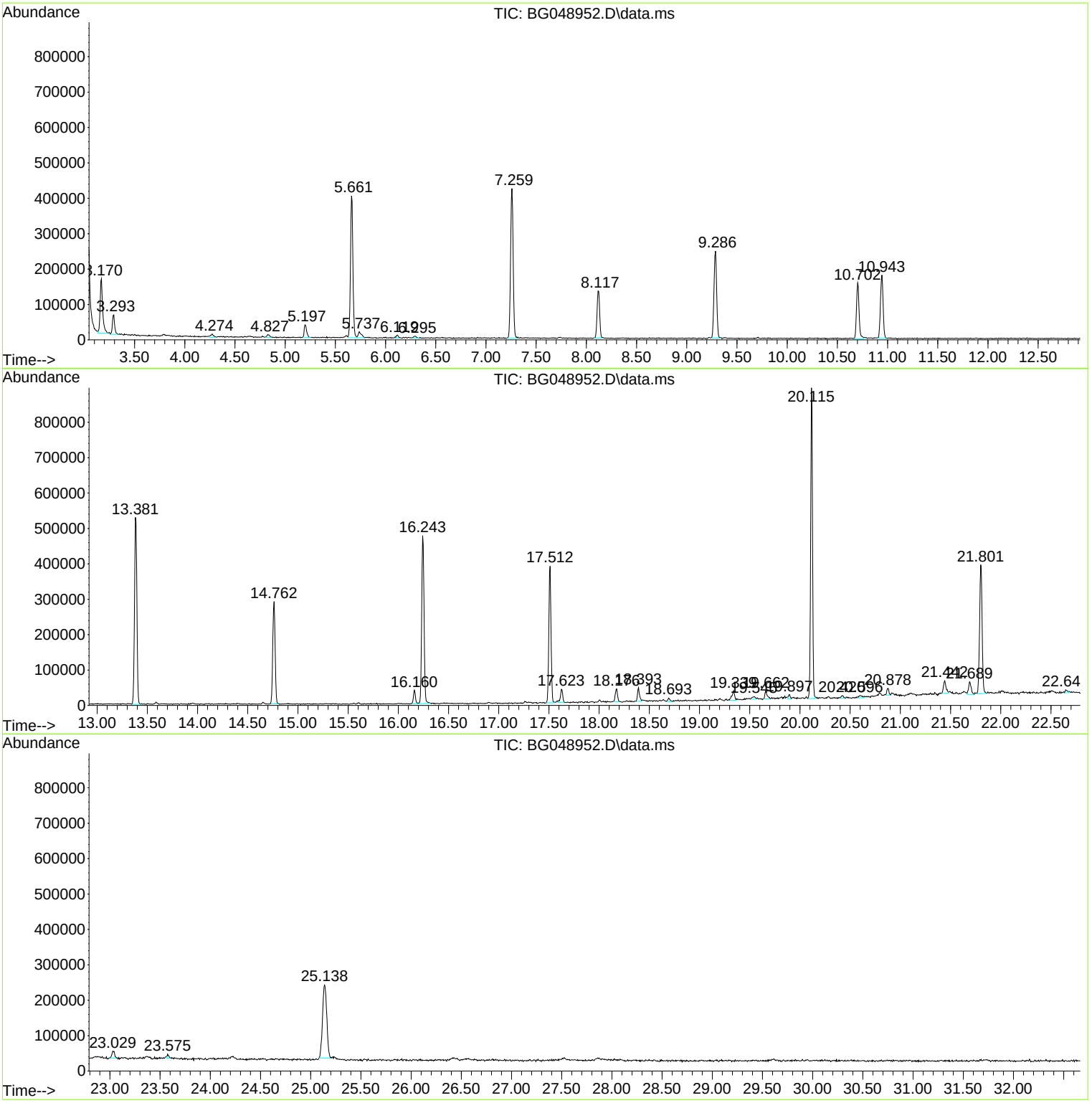
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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Data File : BG048952.D
Acq On : 14 Jun 2021 16:47
Operator : CG/JU
Sample : M2687-08
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
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DUP-01

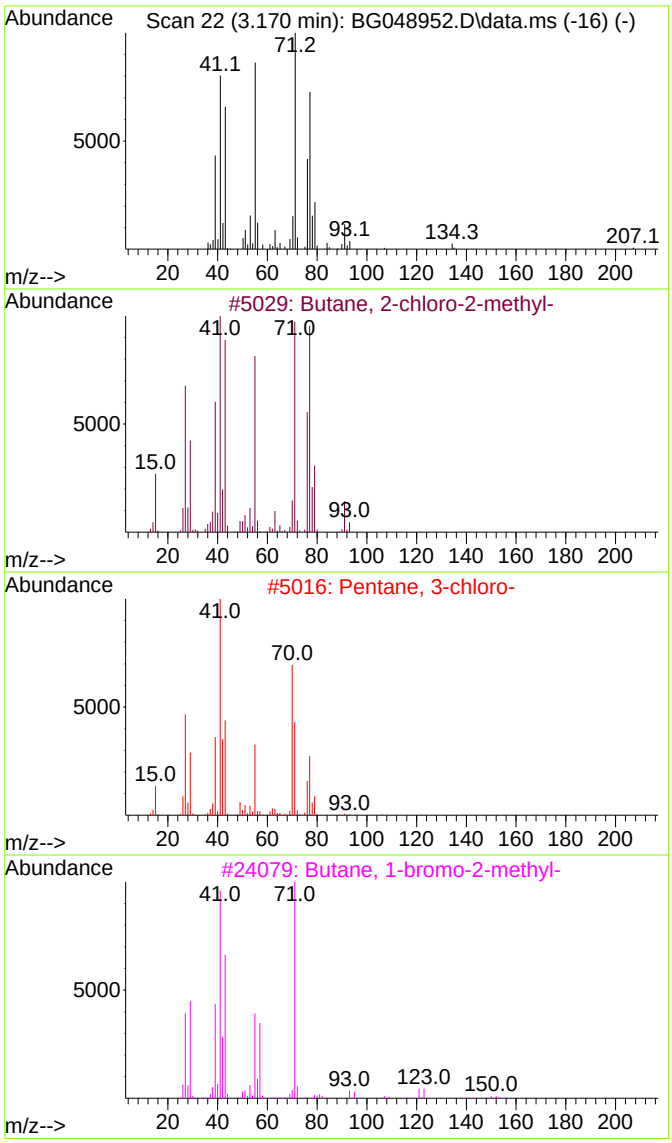
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

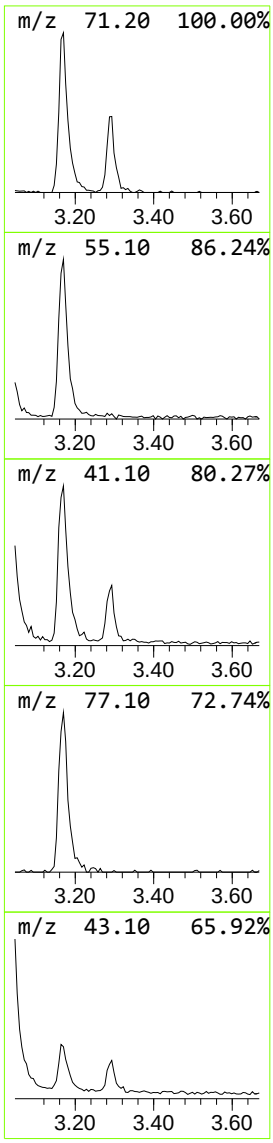
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.170	22.55 ng	266176	1,4-Dichlorobenzene-d4	8.123

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-chloro-2-methyl-	106	C5H11Cl	000594-36-5	59
2	Pentane, 3-chloro-	106	C5H11Cl	000616-20-6	36
3	Butane, 1-bromo-2-methyl-	150	C5H11Br	005973-11-5	25
4	2-Butene, 1-butoxy-3-methyl-	142	C9H18O	022094-02-6	22
5	Oxalic acid, hexyl neopentyl ester	244	C13H24O4	1000309-73-1	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048952.D
Acq On : 14 Jun 2021 16:47
Operator : CG/JU
Sample : M2687-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DUP-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

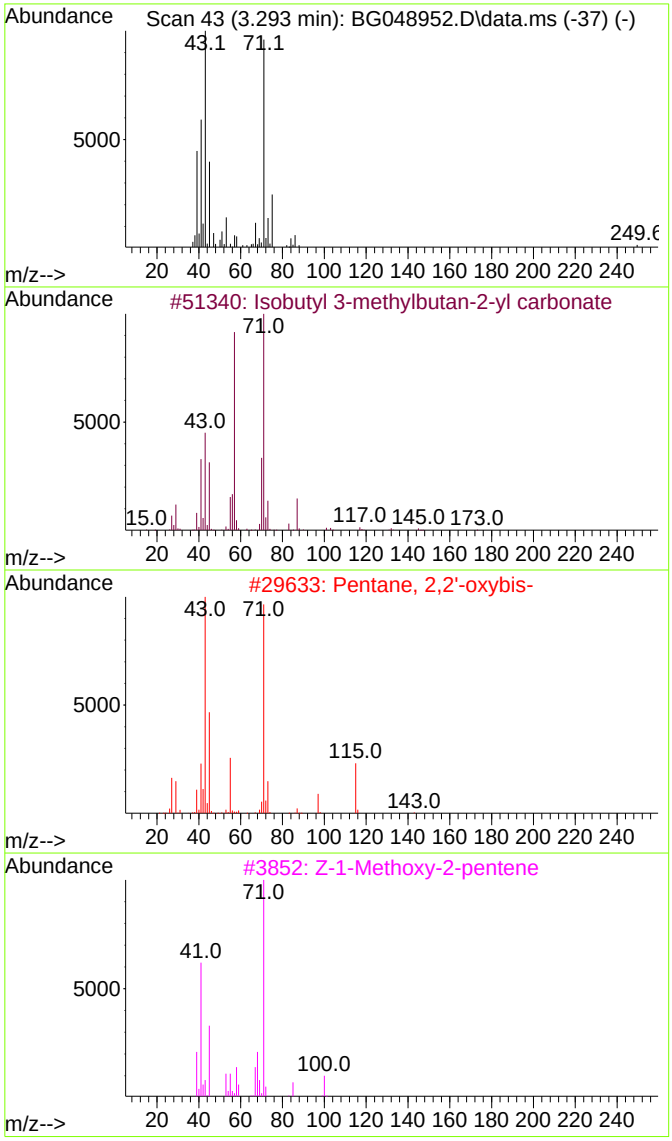
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

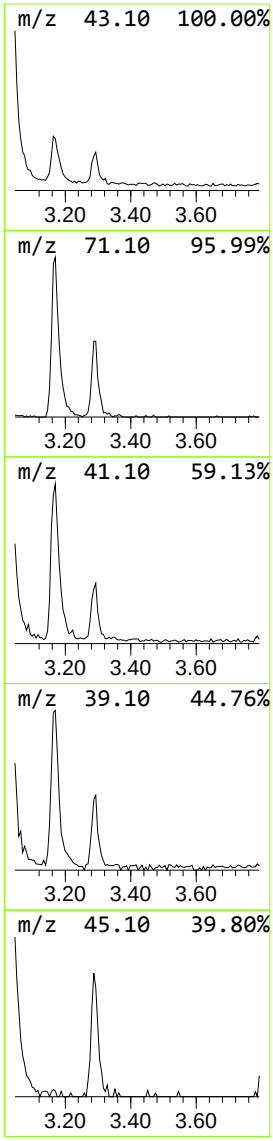
****

Peak Number 2 unknown3.293 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.293	7.15 ng	84374	1,4-Dichlorobenzene-d4	8.123

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl 3-methylbutan-2-yl carb...	188	C10H20O3	1000372-77-0	47
2	Pentane, 2,2'-oxybis-	158	C10H22O	056762-00-6	47
3	Z-1-Methoxy-2-pentene	100	C6H12O	1000279-59-4	43
4	Pantolactone	130	C6H10O3	000599-04-2	42
5	1-Propene, 3-methoxy-2-methyl-	86	C5H10O	022418-49-1	37





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Operator : CG/JU
Sample : M2687-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-01

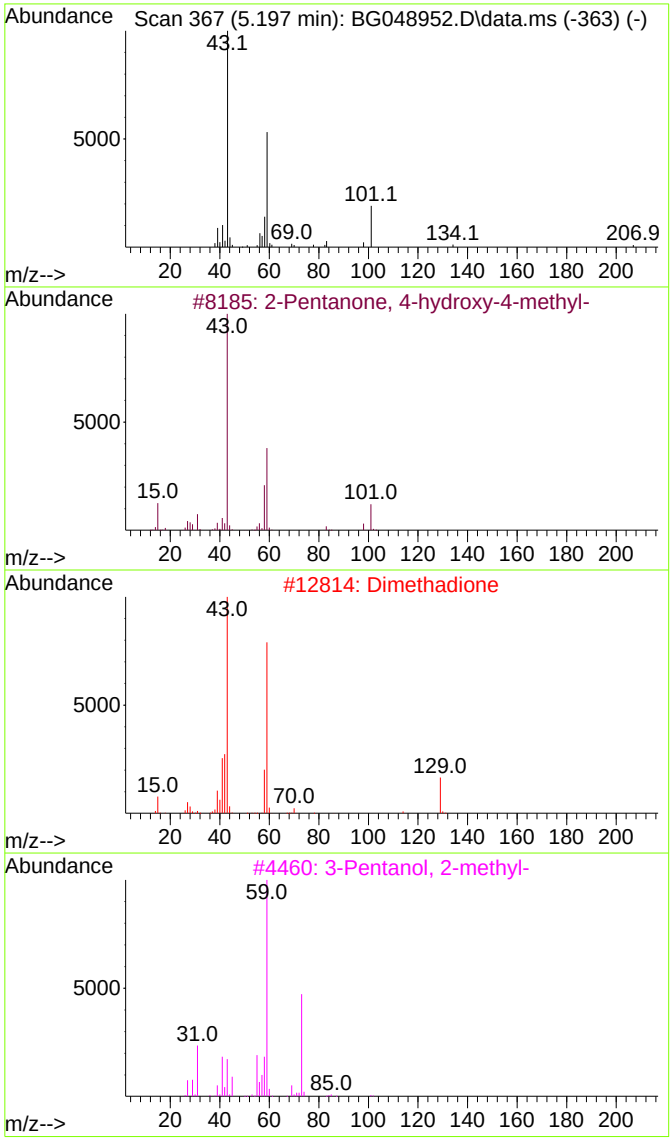
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

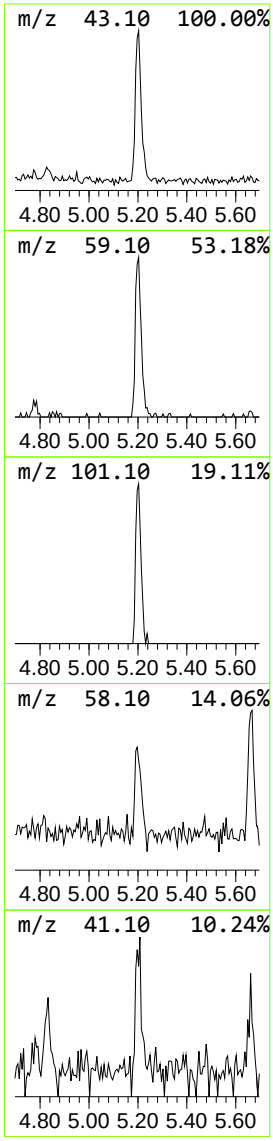
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.197	5.29 ng	62471	1,4-Dichlorobenzene-d4	8.123

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2	Dimethadione	129	C5H7NO3	000695-53-4	33
3	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	32
4	Cycloserine	102	C3H6N2O2	000068-41-7	28
5	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	25





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Operator : CG/JU
Sample : M2687-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

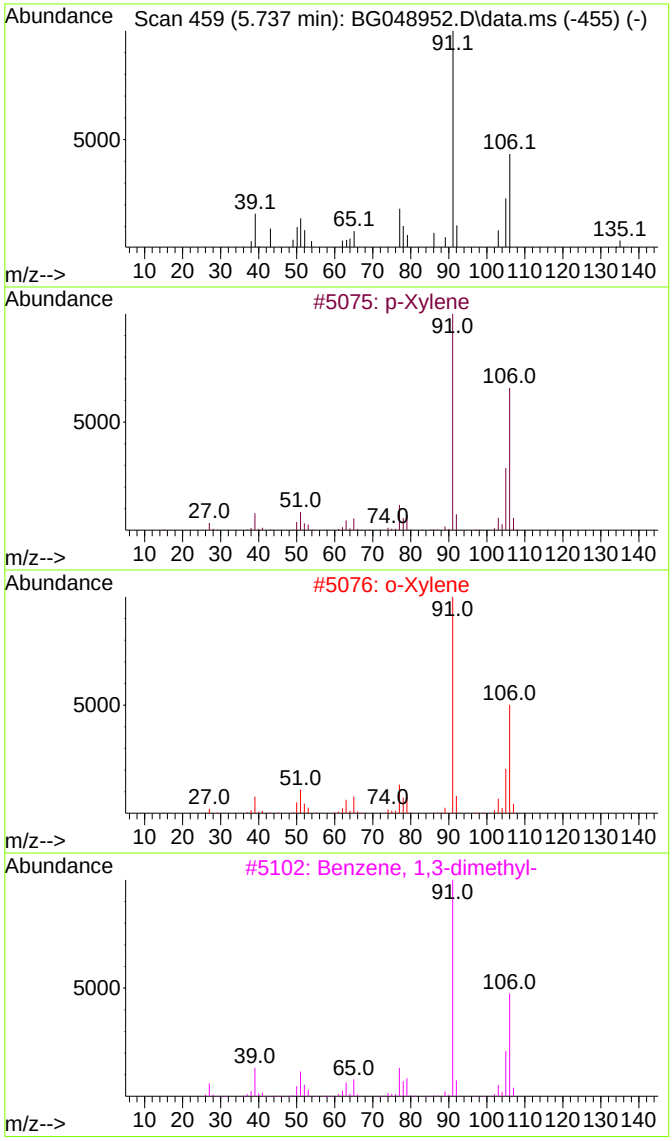
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

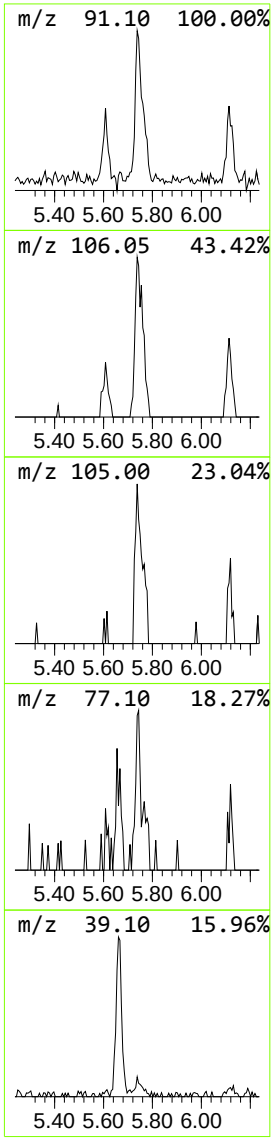
****

Peak Number 4 p-Xylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.737	3.20 ng	37811	1,4-Dichlorobenzene-d4	8.123

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Xylene	106	C8H10	000106-42-3	83
2	o-Xylene	106	C8H10	000095-47-6	80
3	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	80
4	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	64
5	Ethylbenzene	106	C8H10	000100-41-4	64





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DUP-01

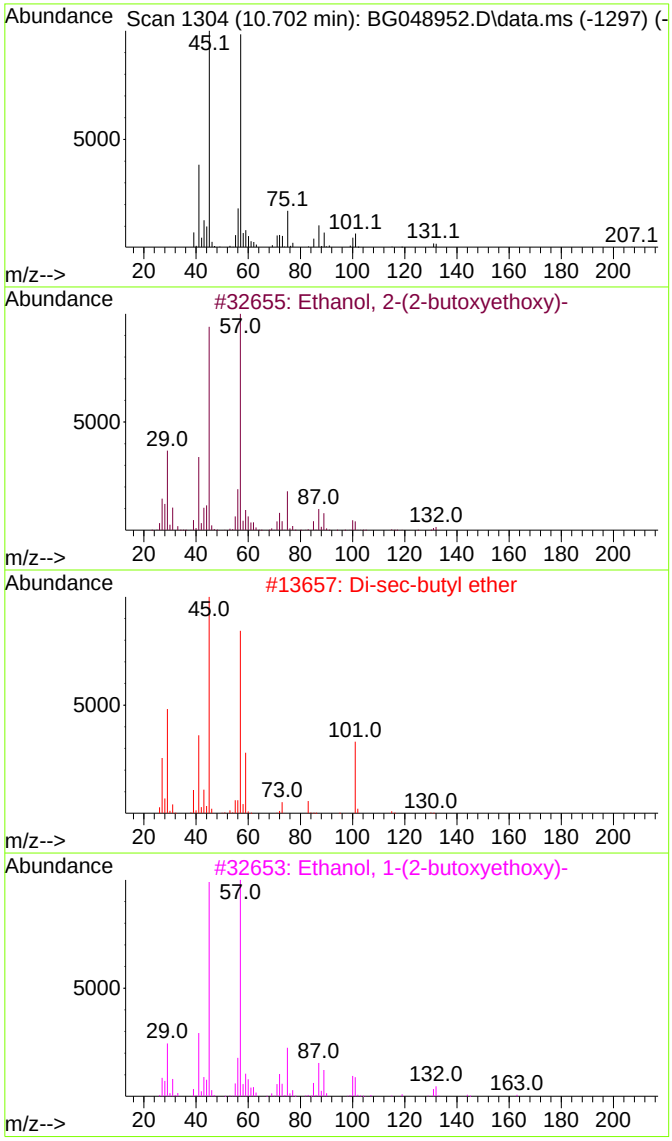
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

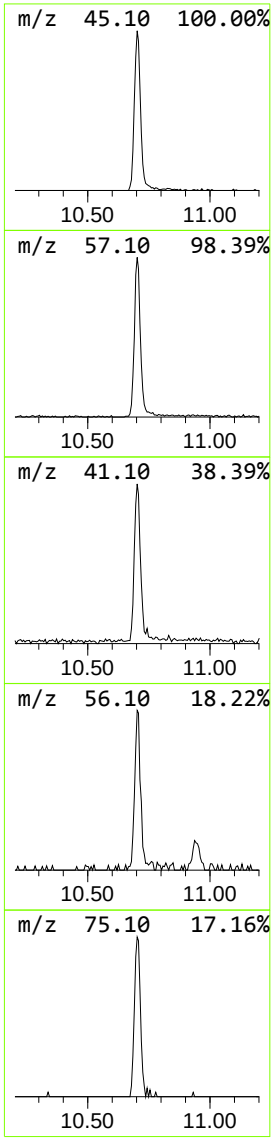
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.702	17.40 ng	282691	Naphthalene-d8	10.943

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Di-sec-butyl ether	130	C8H18O	006863-58-7	59
3	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
4	Hexaethylene glycol monododecyl ...	450	C24H50O7	003055-96-7	50
5	Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	47





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BNA_G
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

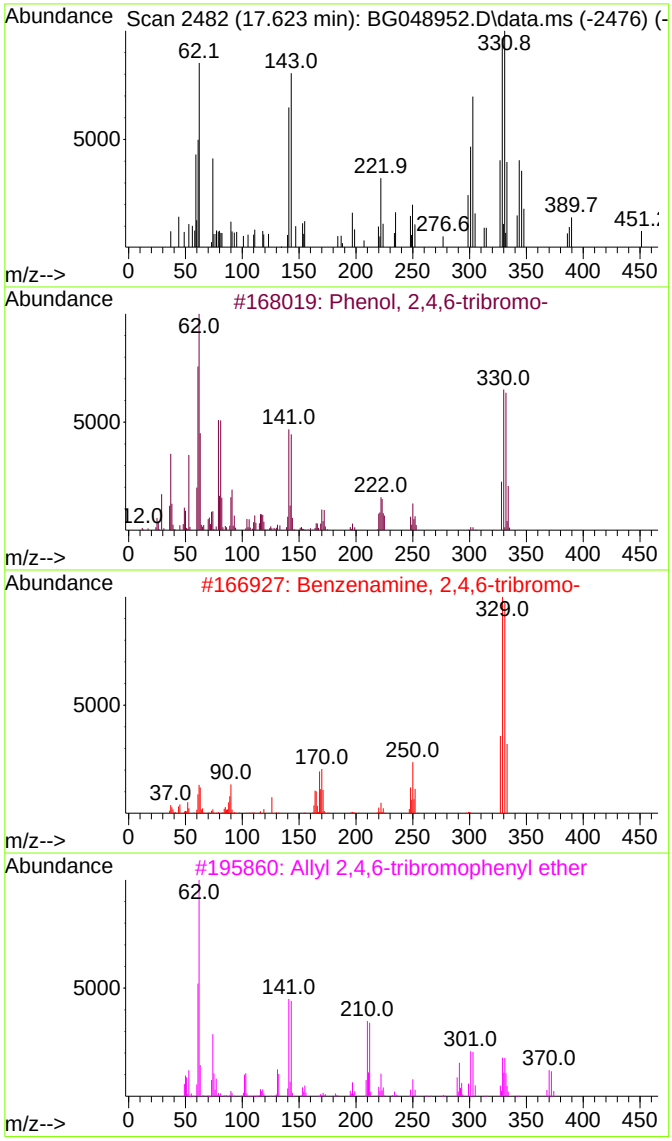
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

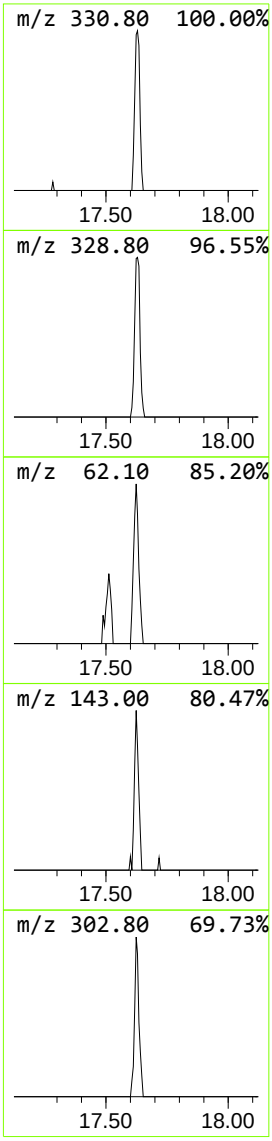
****

Peak Number 6 Benzenamine, 2,4,6-tribromo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.623	2.02 ng	59357	Phenanthrene-d10	17.512

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,4,6-tribromo-	328	C6H3Br3O	000118-79-6	86
2	Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	74
3	Allyl 2,4,6-tribromophenyl ether	368	C9H7Br3O	003278-89-5	23
4	Propylcarbamate	103	C4H9NO2	000627-12-3	16
5	Thiophene, 3,4-dichlorotetrahydr...	188	C4H6Cl2O2S	003001-57-8	12





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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DUP-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

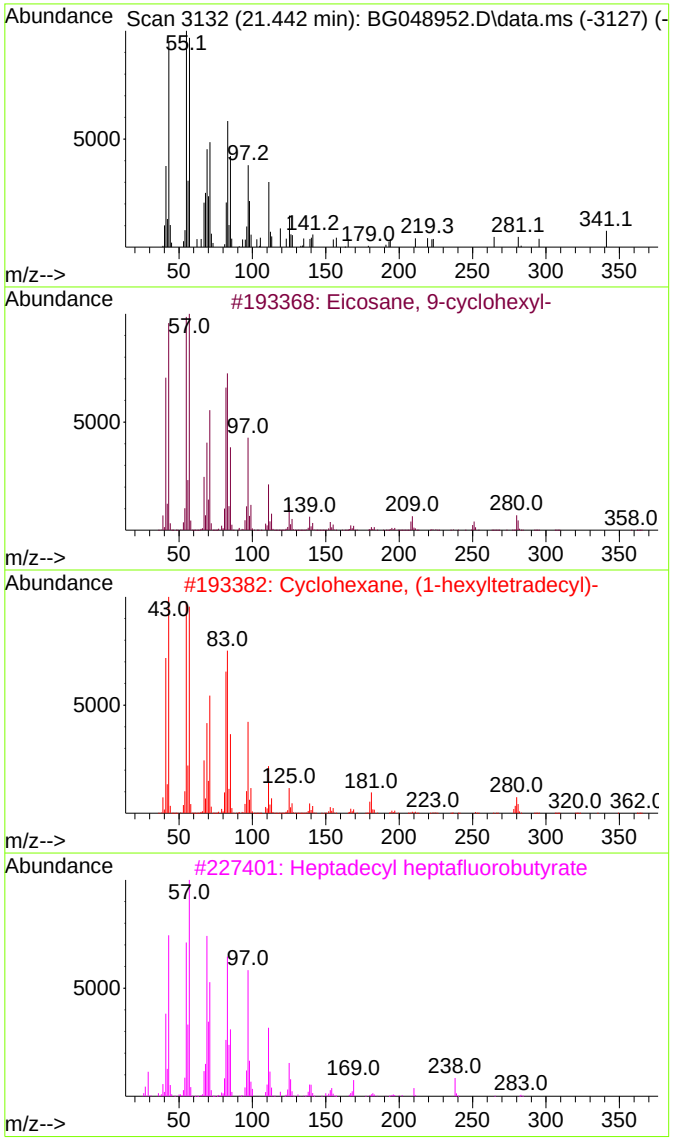
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

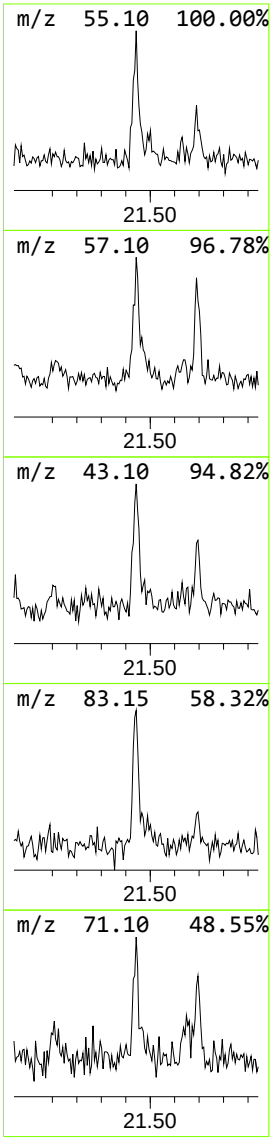
****

Peak Number 7 Eicosane, 9-cyclohexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.442	2.05 ng	65644	Chrysene-d12	21.801

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 9-cyclohexyl-	364	C26H52	004443-61-2	64
2	Cyclohexane, (1-hexyltetradecyl)-	364	C26H52	004443-60-1	64
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	58
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	46
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	46





Tentatively Identified Compound (LSC) summary

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Operator : CG/JU
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ClientSampleId : DUP-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-chlor...	3.170	22.6	ng	266176	1	8.123	236068	20.0
unknown3.293	3.293	7.2	ng	84374	1	8.123	236068	20.0
2-Pentanone, 4-...	5.197	5.3	ng	62471	1	8.123	236068	20.0
p-Xylene	5.737	3.2	ng	37811	1	8.123	236068	20.0
Ethanol, 2-(2-b...	10.702	17.4	ng	282691	2	10.943	324988	20.0
Benzenamine, 2,...	17.623	2.0	ng	59357	4	17.512	587099	20.0
Eicosane, 9-cyc...	21.442	2.0	ng	65644	5	21.801	639998	20.0