LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101519\
Data File : BG043217.D
Acq On : 15 Oct 2019 14:04
Operator : JU
Sample : K5348-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190879-COMPOSITE-K

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-BG092519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.152	6	11	19	rBV4	59699	138921	4.90%	0.854%
2	3.229	19	24	31	rVB	114635	174528	6.16%	1.072%
3	5.156	347	352	361	rBV	68315	109534	3.87%	0.673%
4	5.632	426	433	447	rBV	426732	763715	26.95%	4.693%
5	7.224	695	704	715	rBV	597334	1217015	42.95%	7.478%
6	7.588	756	766	779	rBV	547184	995918	35.15%	6.120%
7	8.053	837	845	852	rBV	169662	309099	10.91%	1.899%
8	8.376	891	900	911	rBV	501717	897178	31.66%	5.513%
9	9.210	1034	1042	1057	rBV	338219	711378	25.11%	4.371%
10	10.855	1315	1322	1338	rBV	202113	420208	14.83%	2.582%
11	12.359	1567	1578	1584	rBV3	13864	36434	1.29%	0.224%
12	13.299	1730	1738	1756	rBV	1011299	1724275	60.85%	10.596%
13	14.122	1869	1878	1888	rBV	150345	242355	8.55%	1.489%
14	14.674	1966	1972	1983	rBV2	376625	648616	22.89%	3.986%
15	16.161	2218	2225	2243	rBV	513936	998333	35.23%	6.135%
16	17.171	2392	2397	2403	rBV6	33328	68542	2.42%	0.421%
17	17.418	2433	2439	2453	rBV2	477408	872327	30.79%	5.360%
18	17.536	2454	2459	2469	rVB4	72862	123474	4.36%	0.759%
19	18.305	2585	2590	2595	rBV6	23304	44345	1.57%	0.272%
20	19.474	2783	2789	2793	rBV	32719	58311	2.06%	0.358%
21	19.833	2846	2850	2859	rVB2	40404	73078	2.58%	0.449%
22	20.027	2877	2883	2895	rBV	1992776	2833541	100.00%	17.412%
23	20.326	2930	2934	2938	rVB7	18854	29949	1.06%	0.184%
24	20.826	3015	3019	3026	rBV8	21294	32522	1.15%	0.200%
25	21.331	3100	3105	3116	rBV2	87422	190119	6.71%	1.168%
26	21.695	3159	3167	3183	rVB	541930	1118189	39.46%	6.871%
27	21.883	3195	3199	3205	rVB4	27701	39561	1.40%	0.243%
28	22.494	3299	3303	3307	rVB4	27434	36065	1.27%	0.222%
29	23.188	3415	3421	3429	rVB3	29864	63425	2.24%	0.390%
30	23.376	3449	3453	3459	rVB5	27512	52714	1.86%	0.324%
31	23.993	3555	3558	3567	rVB5	34701	65158	2.30%	0.400%
32	24.762	3684	3689	3696	rBV2	14864	39169	1.38%	0.241%
33	24.915	3705	3715	3735	rBV3	364503	1145536	40.43%	7.039%

LSC Area Percent Report

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Acq On : 15 Oct 2019 14:04
Operator : JU
Sample : K5348-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190879-COMPOSITE-K

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-BG092519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

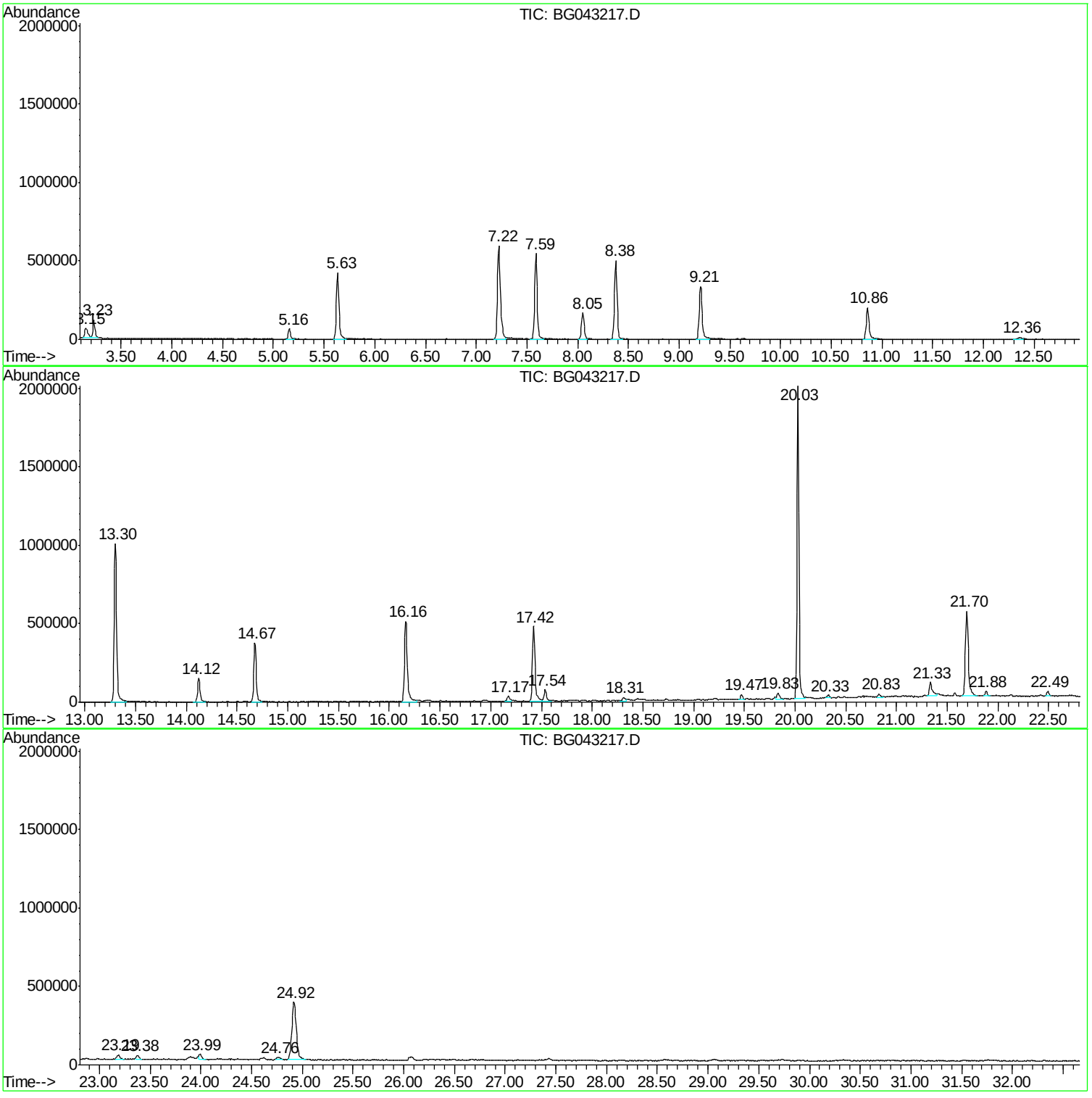
Sum of corrected areas: 16273532

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101519\
Data File : BG043217.D
Acq On : 15 Oct 2019 14:04
Operator : JU
Sample : K5348-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20190879-COMPOSITE-K

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101519\
Data File : BG043217.D
Acq On : 15 Oct 2019 14:04
Operator : JU
Sample : K5348-11
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ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190879-COMPOSITE-K

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

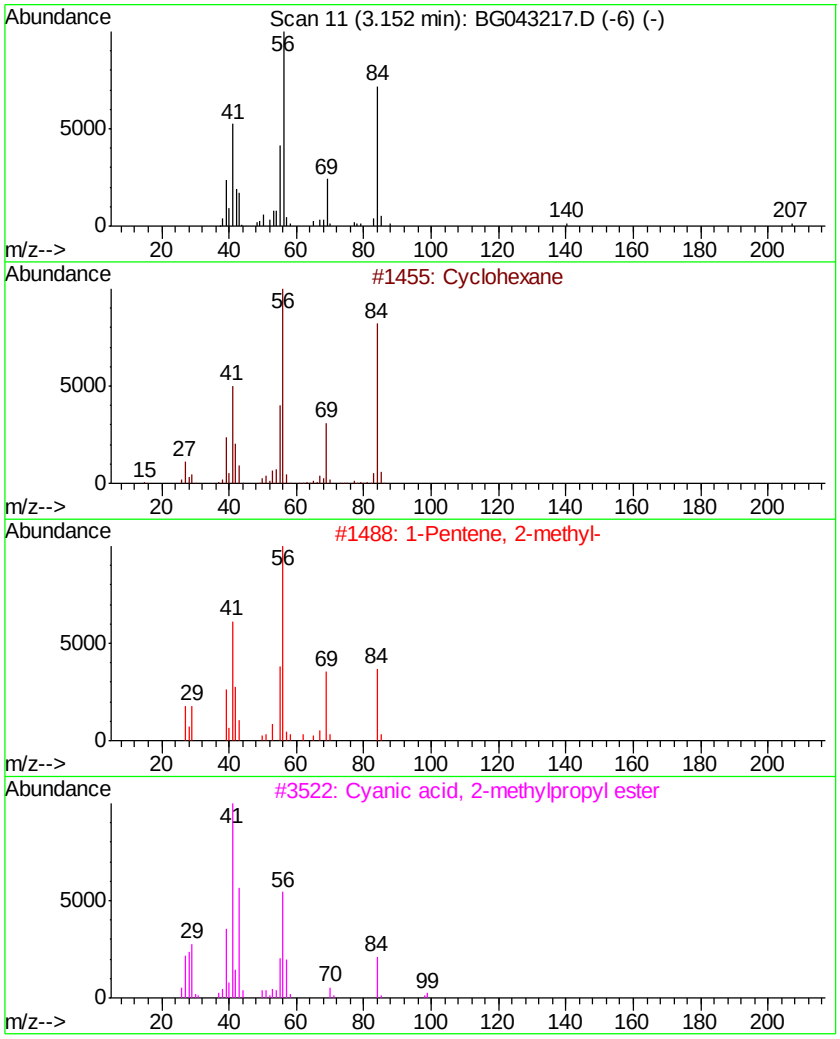
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

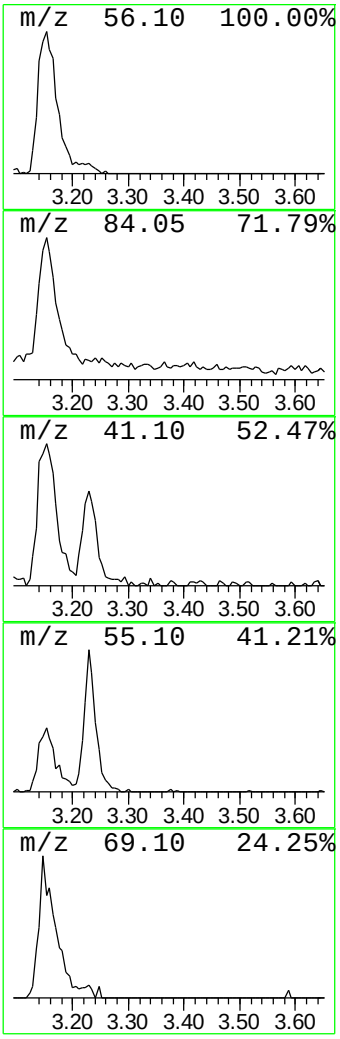
****

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.15	8.99 ng	138921	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	90
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	78
3	Cyanic acid, 2-methylpropyl ester	99	C5H9NO	001768-25-8	64
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	50
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	47





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101519\
Data File : BG043217.D
Acq On : 15 Oct 2019 14:04
Operator : JU
Sample : K5348-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190879-COMPOSITE-K

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

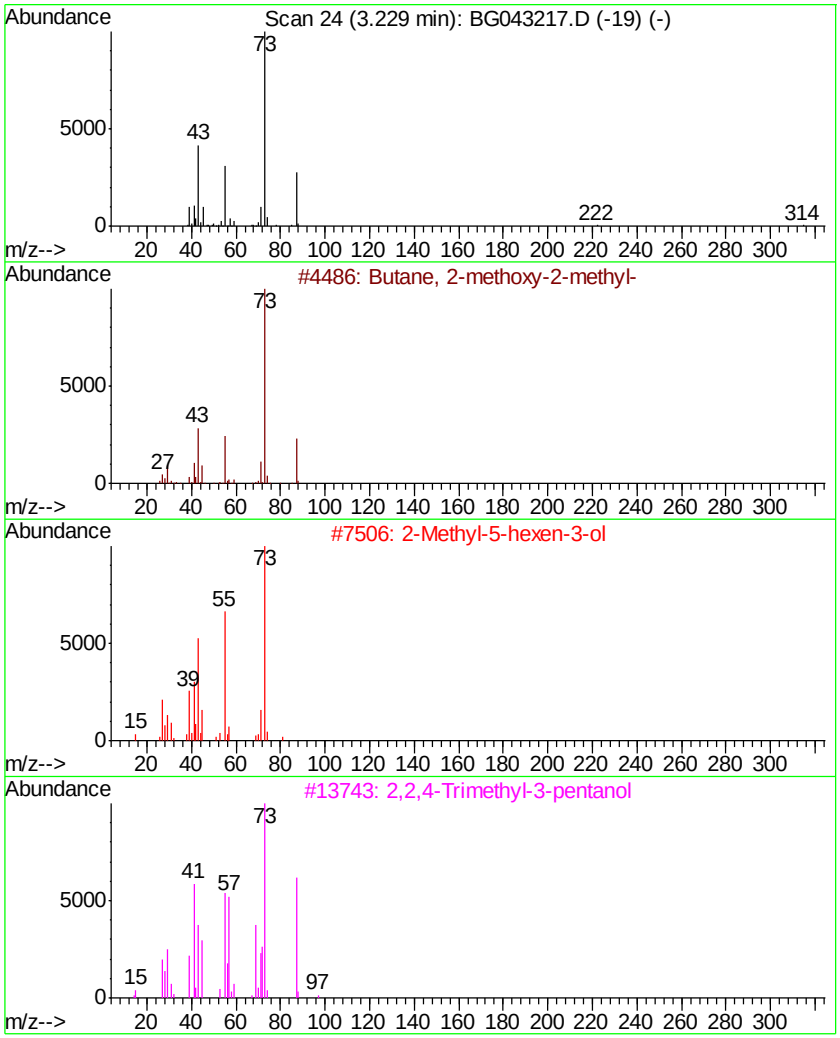
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

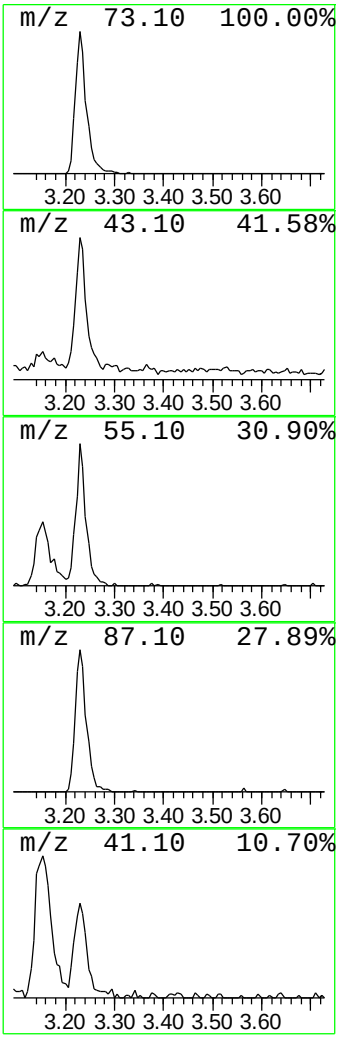
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	11.29 ng	174528	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101519\
Data File : BG043217.D
Acq On : 15 Oct 2019 14:04
Operator : JU
Sample : K5348-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190879-COMPOSITE-K

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

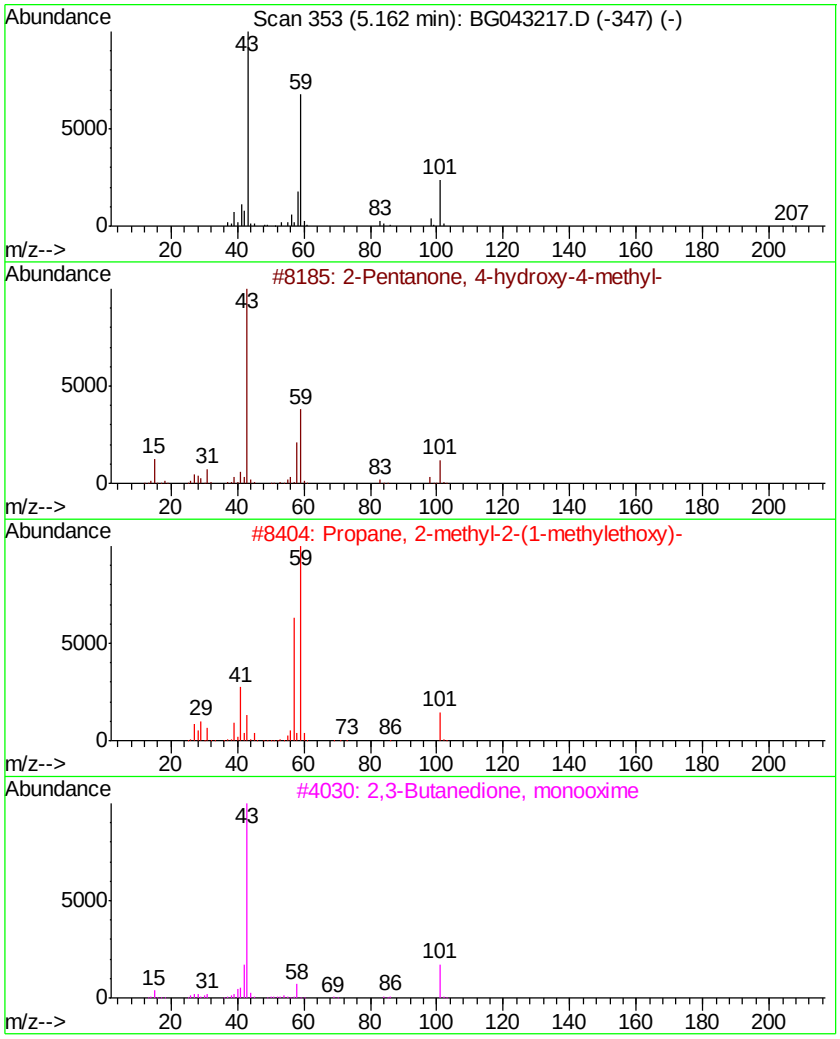
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

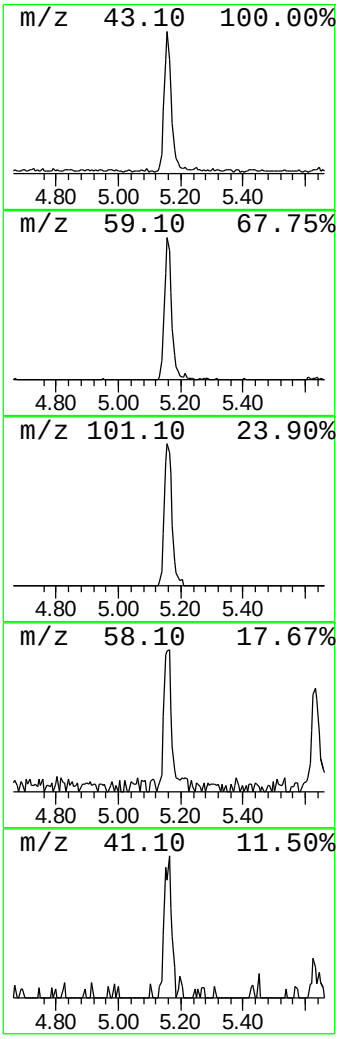
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	7.09 ng	109534	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	40
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
5	1,2-Butanediol	90	C4H10O2	000584-03-2	23





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101519\
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Acq On : 15 Oct 2019 14:04
Operator : JU
Sample : K5348-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190879-COMPOSITE-K

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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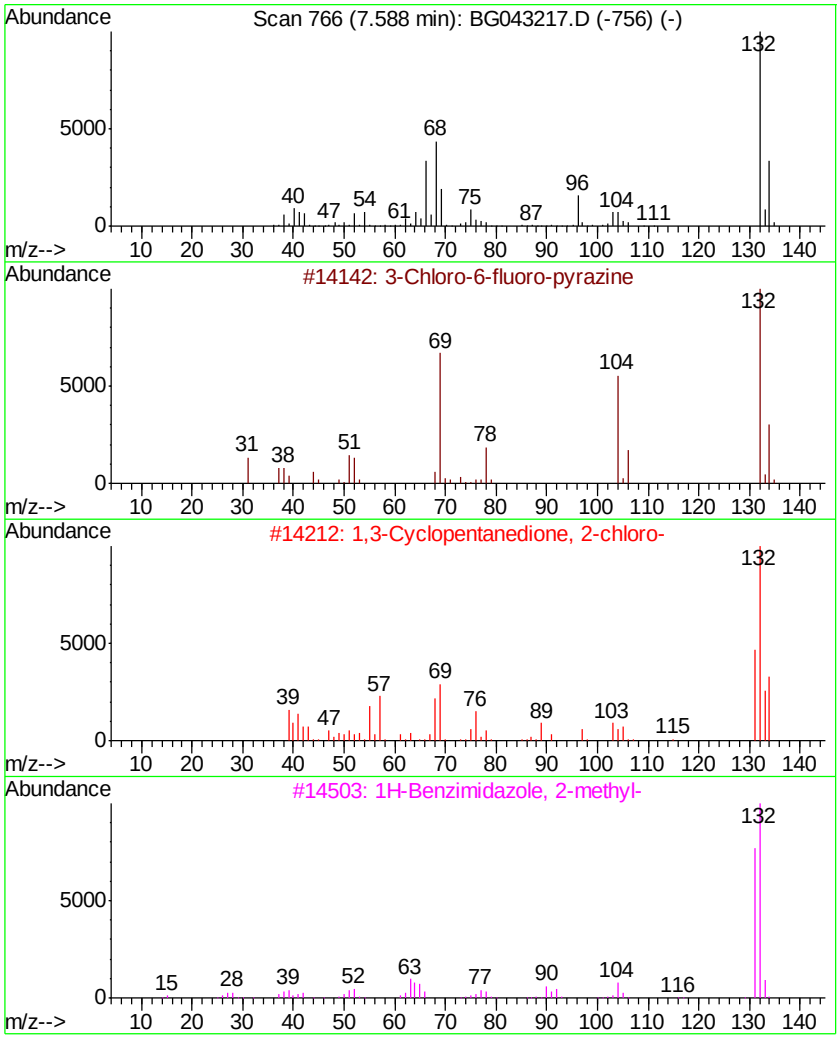
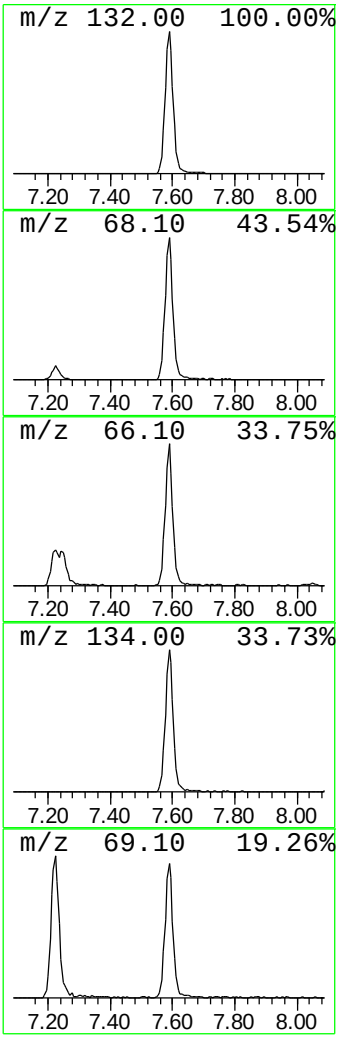
****

Peak Number 4 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	64.44 ng	995918	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	16
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101519\
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ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20190879-COMPOSITE-K

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

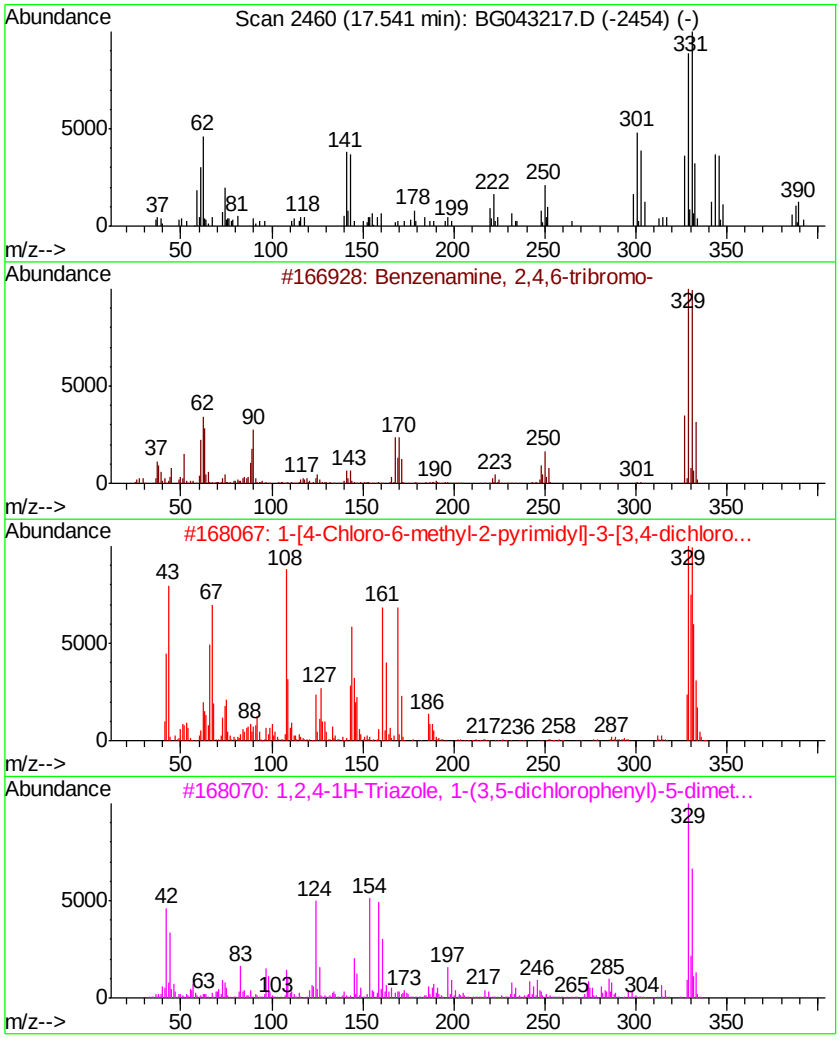
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

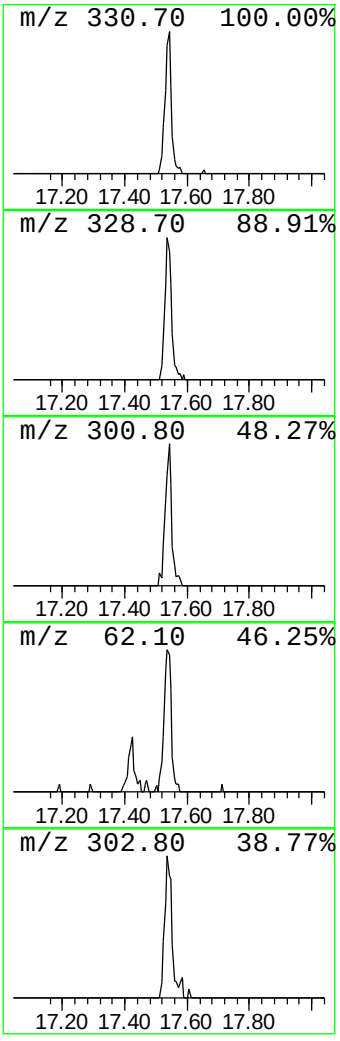
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.54	2.83 ng	123474	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	55
2	1-[4-Chloro-6-methyl-2-pyrimidyl...	329	C12H10Cl3N5	051387-79-2	22
3	1,2,4-1H-Triazole, 1-(3,5-dichlo...	329	C12H13Cl2N5S	1000266-38-9	18
4	Bromophos	364	C8H8BrCl2O3PS	002104-96-3	12
5	4',7-Dichloro-6-methyl cinchophen	331	C17H11Cl2NO2	1000256-43-4	11





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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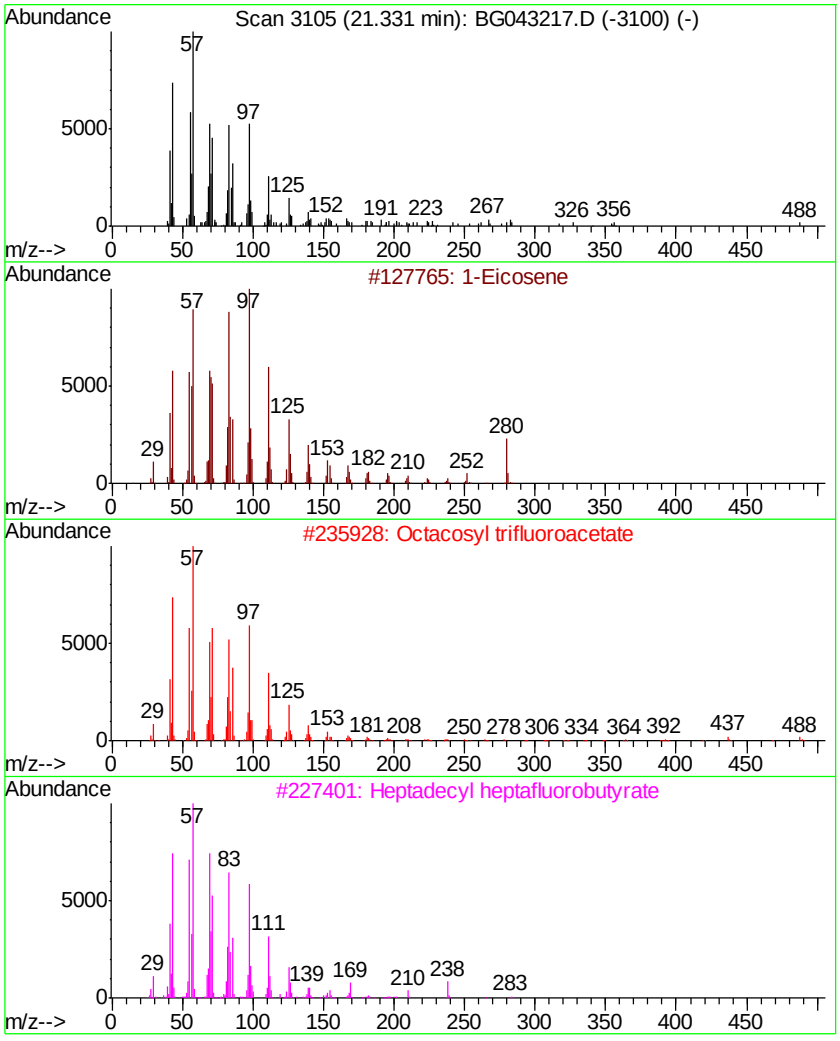
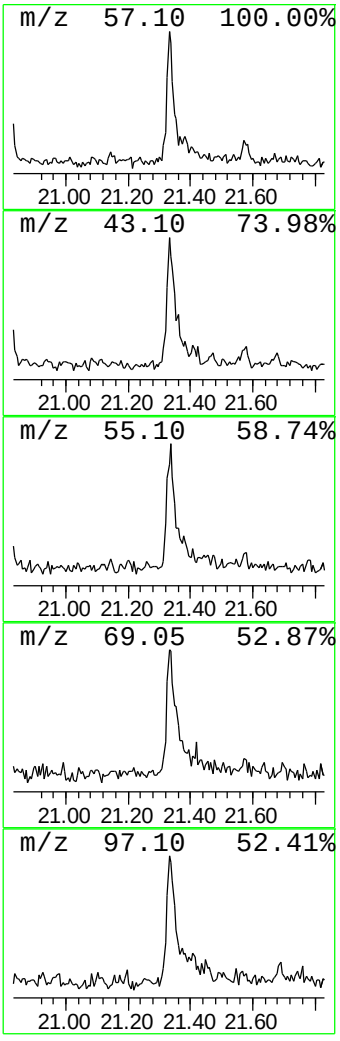
****

Peak Number 7 1-Eicosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.33	3.40 ng	190119	Chrysene-d12	21.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosene	280	C20H40	003452-07-1	97
2	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91





Tentatively Identified Compound (LSC) summary

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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
1-Pentene, 2-methyl-	3.15	9.0	ng	138921	1	8.05	309099	20.0
Butane, 2-methoxy...	3.23	11.3	ng	174528	1	8.05	309099	20.0
2-Pentanone, 4-hy...	5.16	7.1	ng	109534	1	8.05	309099	20.0
unknown7.59	7.59	64.4	ng	995918	1	8.05	309099	20.0
Benzenamine, 2,4,...	17.54	2.8	ng	123474	4	17.42	872327	20.0
1-Eicosene	21.33	3.4	ng	190119	5	21.70	1118190	20.0