LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
Data File : BG043475.D
Acq On : 1 Nov 2019 21:10
Operator : JU
Sample : K5143-05 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NB-08-103019

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-BG102119.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	3.194	12	18	26	rVB2	51976	105093	7.67%	0.883%
2	5.121	341	346	354	rBV	66880	107234	7.83%	0.901%
3	5.603	421	428	443	rBV	319836	594125	43.37%	4.991%
4	7.195	688	699	716	rBV	322695	664097	48.48%	5.578%
5	7.554	751	760	777	rBV	361451	674048	49.21%	5.662%
6	8.012	831	838	847	rBV	180377	327360	23.90%	2.750%
7	8.335	887	893	905	rBV	280804	521009	38.04%	4.377%
8	9.175	1029	1036	1053	rBV	178128	389591	28.44%	3.273%
9	10.820	1309	1316	1327	rBV	211874	426228	31.12%	3.580%
10	13.265	1724	1732	1755	rBV	539284	936533	68.37%	7.867%
11	14.093	1864	1873	1885	rBV	85543	146696	10.71%	1.232%
12	14.639	1960	1966	1975	rBV	375518	629281	45.94%	5.286%
13	16.132	2213	2220	2239	rBV	455641	803298	58.64%	6.748%
14	17.383	2426	2433	2439	rBV	432354	731914	53.43%	6.148%
15	17.507	2448	2454	2462	rVB8	8349	18098	1.32%	0.152%
16	18.047	2541	2546	2552	rBV2	66743	92242	6.73%	0.775%
17	18.276	2579	2585	2590	rBV5	40650	71388	5.21%	0.600%
18	19.181	2734	2739	2742	rBV	191888	260422	19.01%	2.188%
19	19.211	2742	2744	2757	rVB2	297812	401123	29.28%	3.369%
20	19.346	2763	2767	2771	rVB	38350	47371	3.46%	0.398%
21	19.440	2777	2783	2788	rBV	50456	79818	5.83%	0.670%
22	19.769	2835	2839	2841	rBV4	14228	19738	1.44%	0.166%
23	19.798	2841	2844	2851	rVB2	50506	75407	5.51%	0.633%
24	19.998	2872	2878	2889	rBV	979037	1369785	100.00%	11.506%
25	20.297	2926	2929	2932	rVB5	14810	17809	1.30%	0.150%
26	20.439	2950	2953	2956	rBV5	13716	20163	1.47%	0.169%
27	20.791	3010	3013	3016	rVB4	15923	18654	1.36%	0.157%
28	21.296	3095	3099	3107	rVB3	54567	93994	6.86%	0.790%
29	21.655	3152	3160	3174	rVB2	527657	997814	72.84%	8.382%
30	21.843	3188	3192	3195	rVB4	20646	28916	2.11%	0.243%
31	22.442	3290	3294	3300	rVB7	29940	53562	3.91%	0.450%
32	23.317	3438	3443	3448	rVB	41705	75952	5.54%	0.638%
33	23.917	3541	3545	3551	rVB7	35942	82545	6.03%	0.693%
34	24.845	3693	3703	3715	rBV2	341153	1023334	74.71%	8.596%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
Data File : BG043475.D
Acq On : 1 Nov 2019 21:10
Operator : JU
Sample : K5143-05 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NB-08-103019

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-BG102119.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

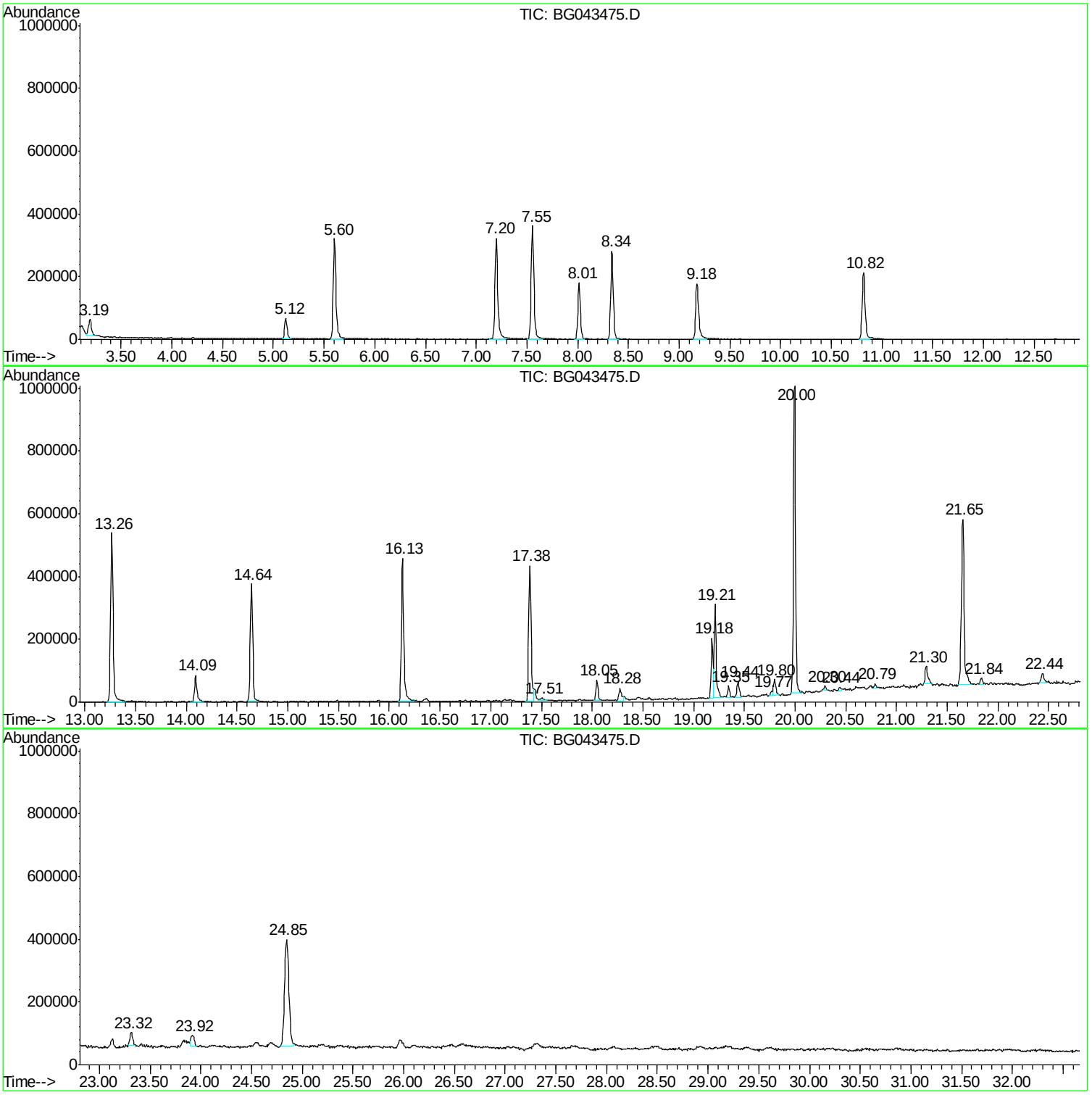
Sum of corrected areas: 11904642

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
Data File : BG043475.D
Acq On : 1 Nov 2019 21:10
Operator : JU
Sample : K5143-05 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NB-08-103019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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\BG110119\
Data File : BG043475.D
Acq On : 1 Nov 2019 21:10
Operator : JU
Sample : K5143-05 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NB-08-103019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

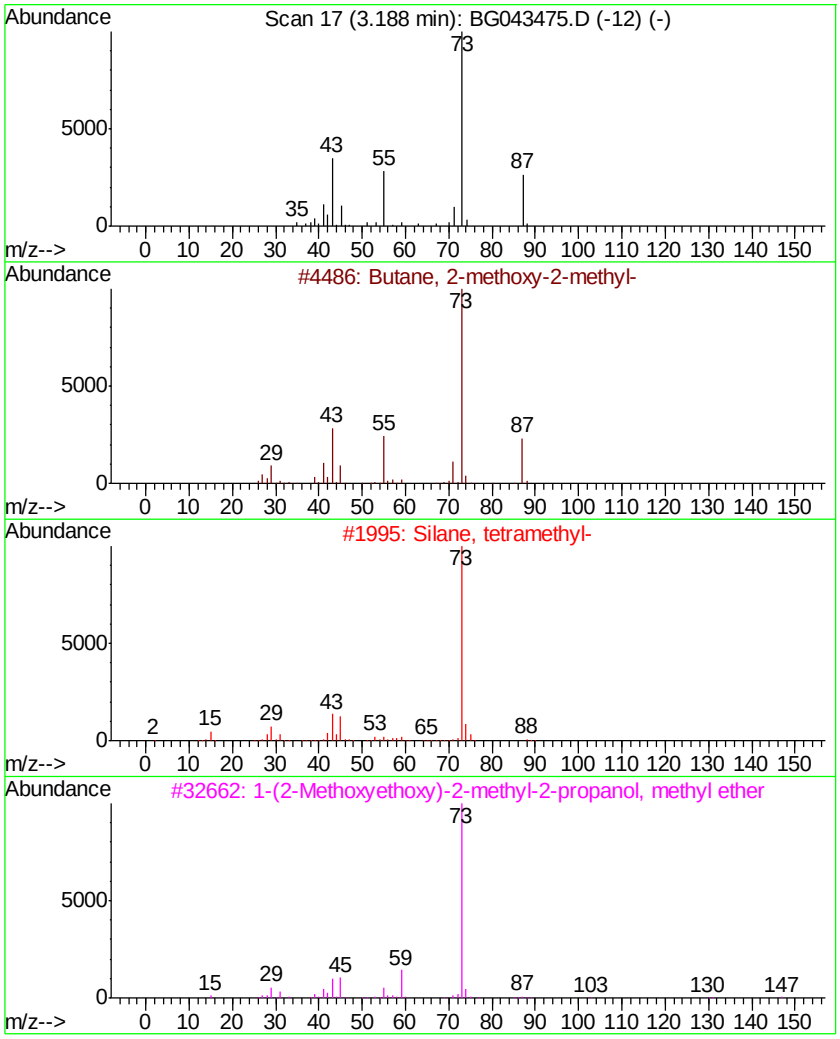
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

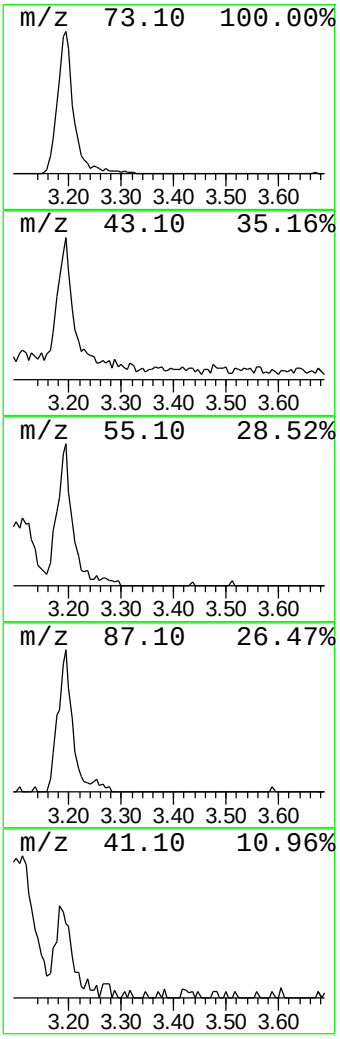
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	6.42 ng	105093	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	1-Propene-1-thiol	74	C3H6S	000925-89-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
Data File : BG043475.D
Acq On : 1 Nov 2019 21:10
Operator : JU
Sample : K5143-05 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NB-08-103019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

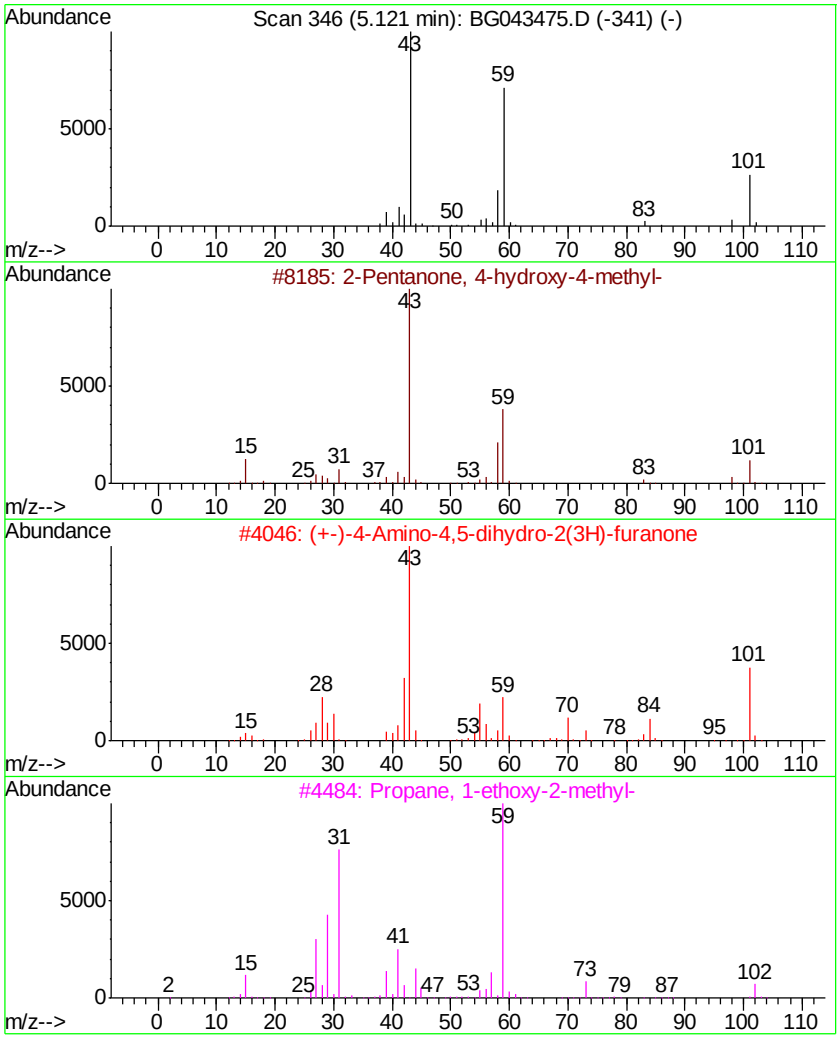
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

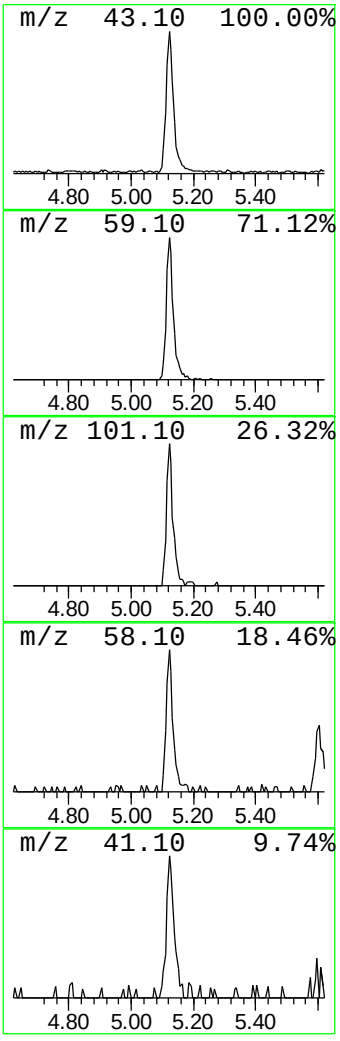
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	6.55 ng	107234	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	37
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	17
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	16





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
Data File : BG043475.D
Acq On : 1 Nov 2019 21:10
Operator : JU
Sample : K5143-05 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NB-08-103019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

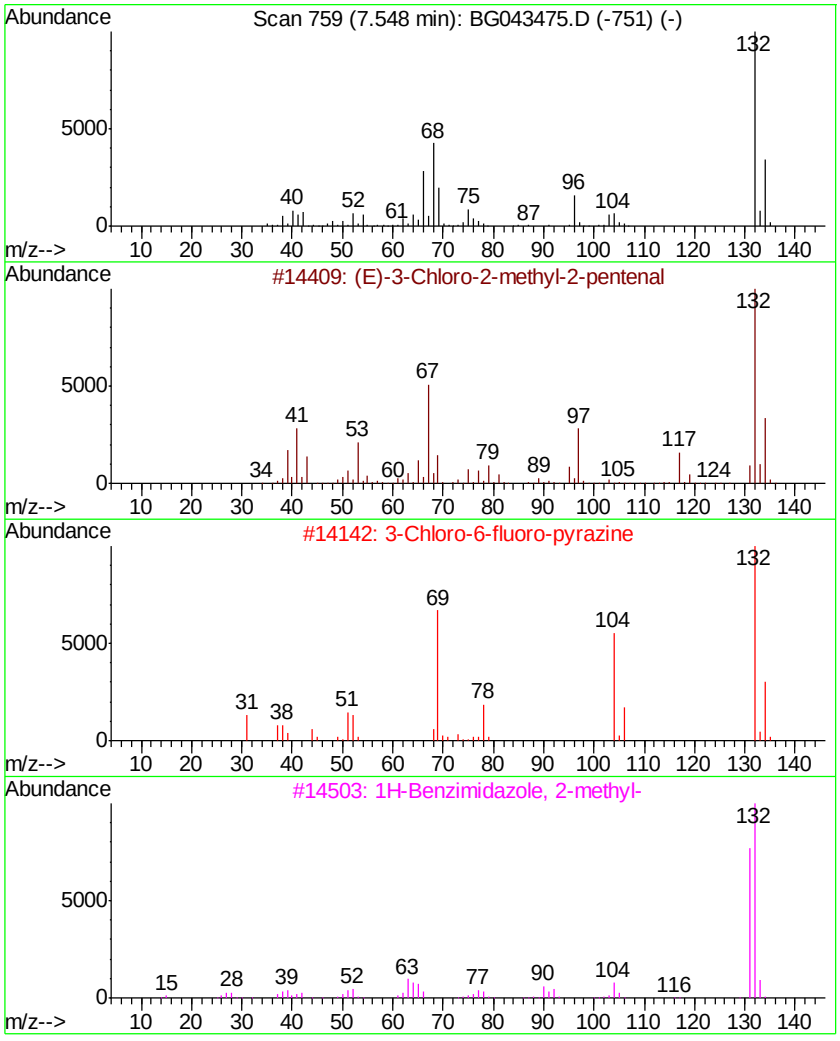
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

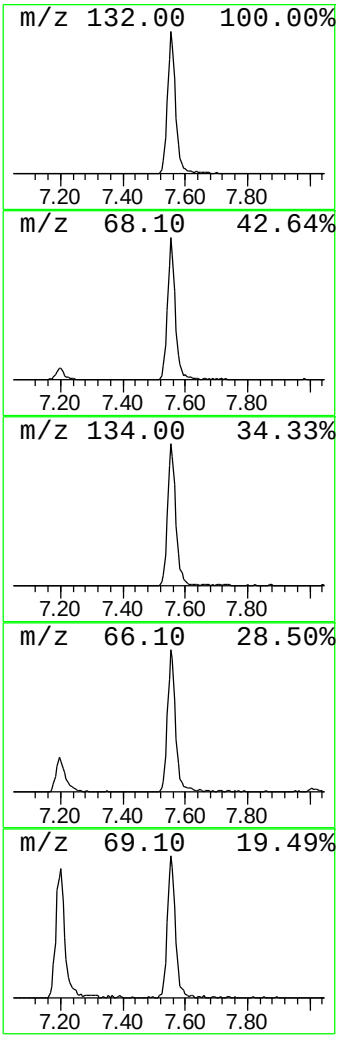
****

Peak Number 3 unknown7.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	41.18 ng	674048	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	30
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
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Acq On : 1 Nov 2019 21:10
Operator : JU
Sample : K5143-05 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NB-08-103019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

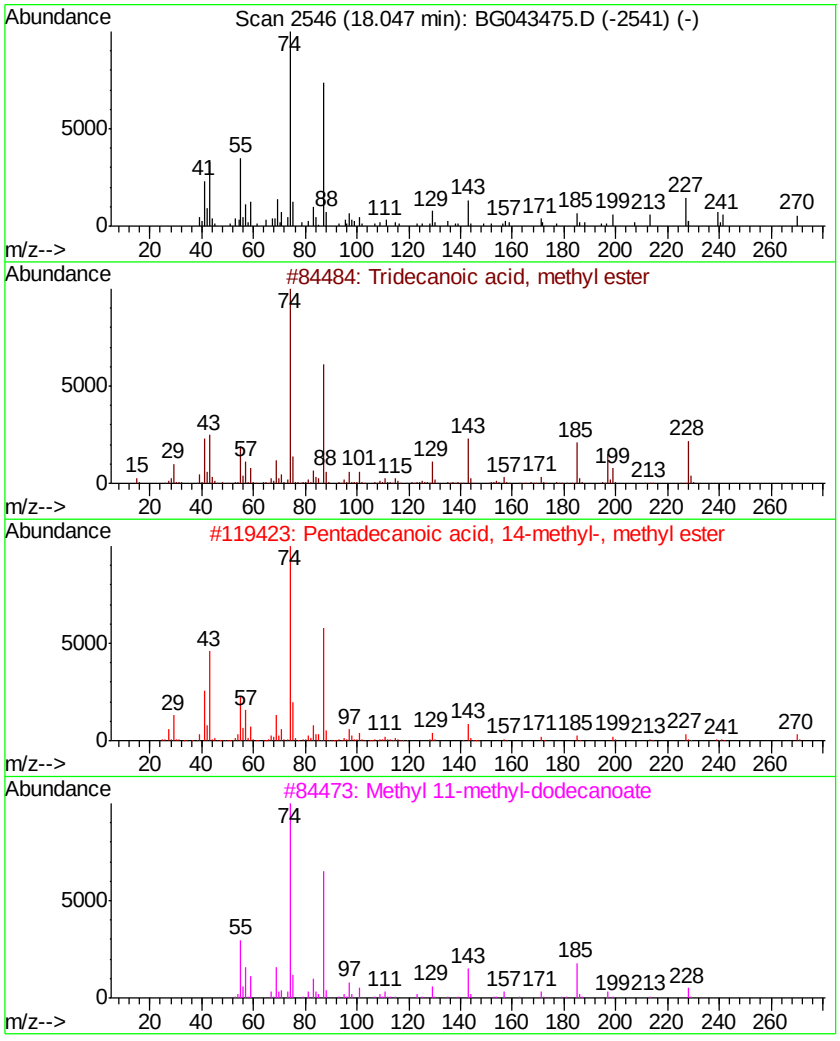
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

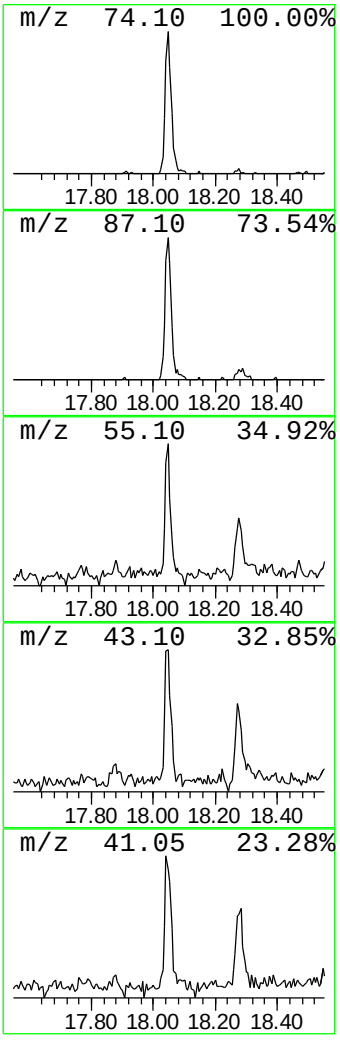
****

Peak Number 5 Tridecanoic acid, methyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.05	2.52 ng	92242	Phenanthrene-d10	17.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	91
4	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	87
5	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NB-08-103019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

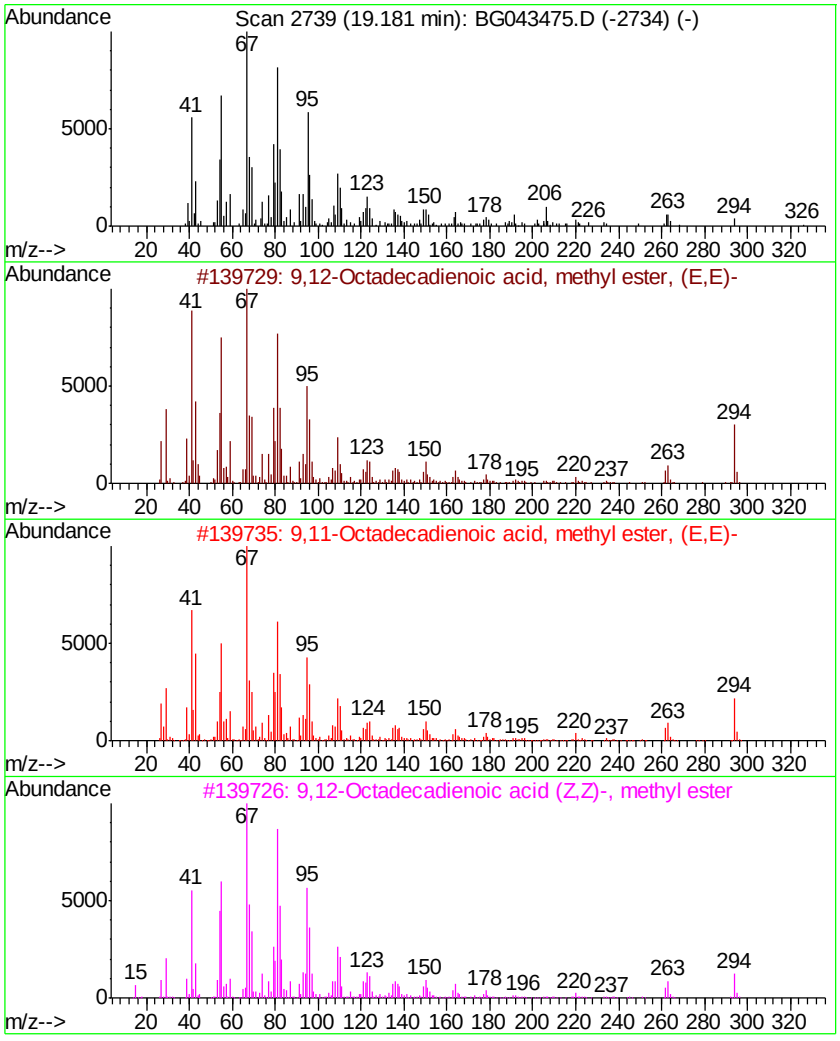
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

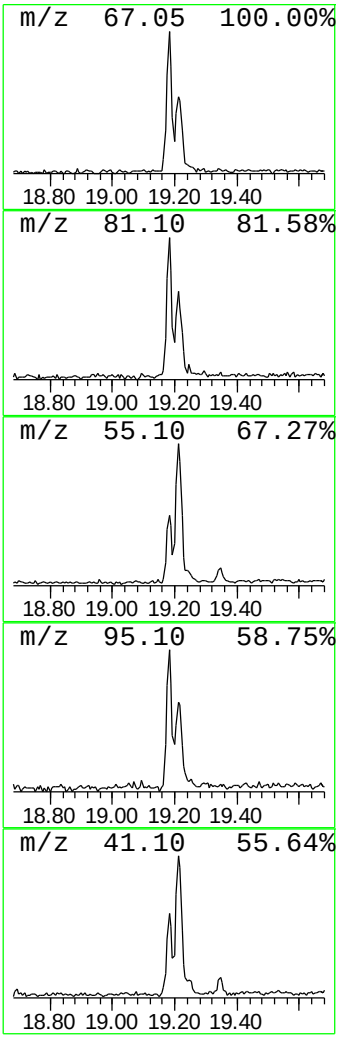
****

Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.18	7.12 ng	260422	Phenanthrene-d10	17.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	99
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98
4	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	97
5	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	97





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
Data File : BG043475.D
Acq On : 1 Nov 2019 21:10
Operator : JU
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NB-08-103019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

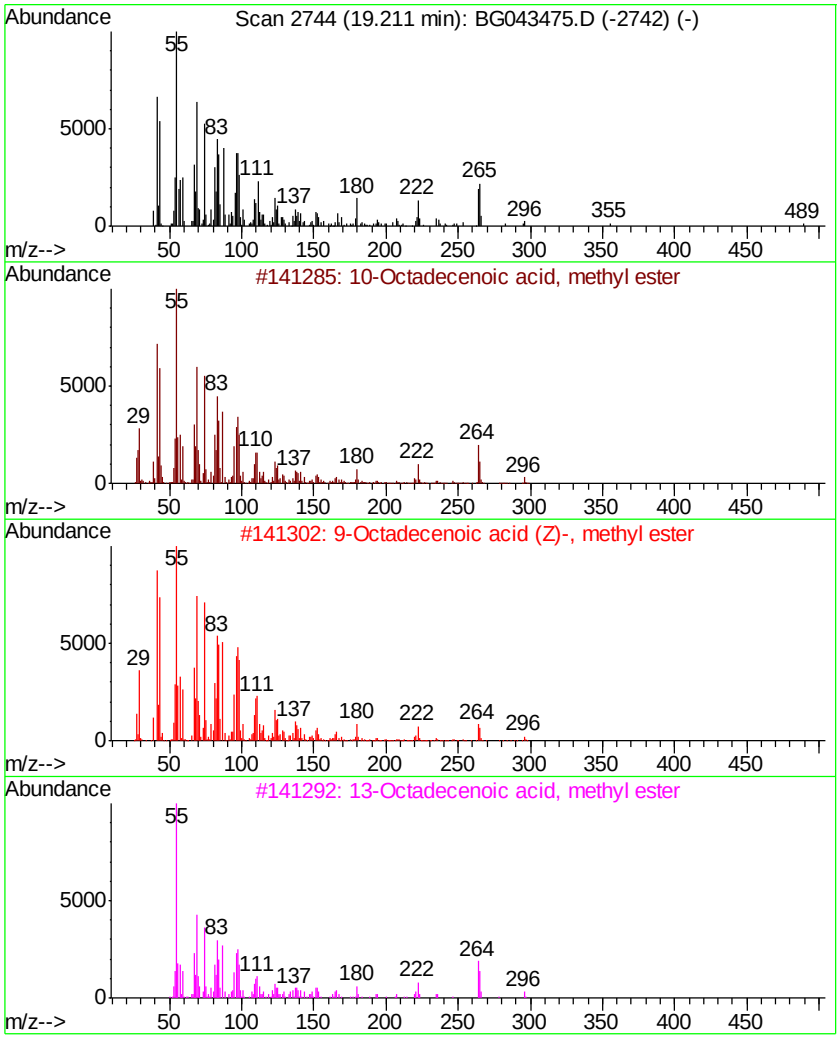
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

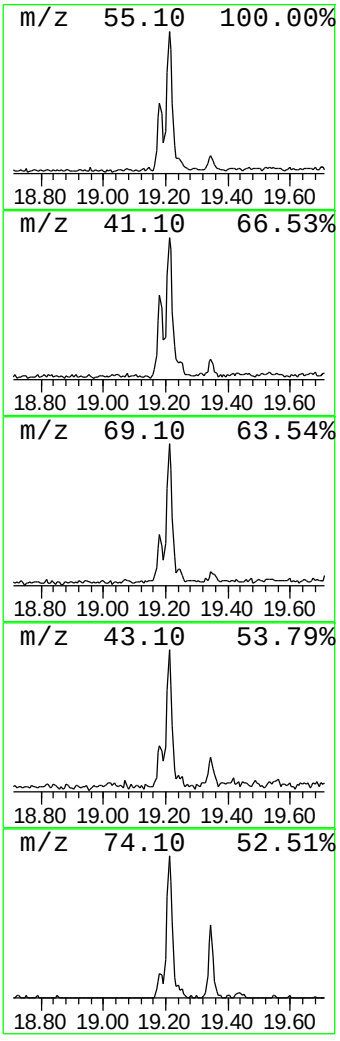
****

Peak Number 7 10-Octadecenoic acid, methy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.21	10.96 ng	401123	Phenanthrene-d10	17.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	98
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	96
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	96
4	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	95
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	95





Library Search Compound Report

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Data File : BG043475.D
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NB-08-103019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

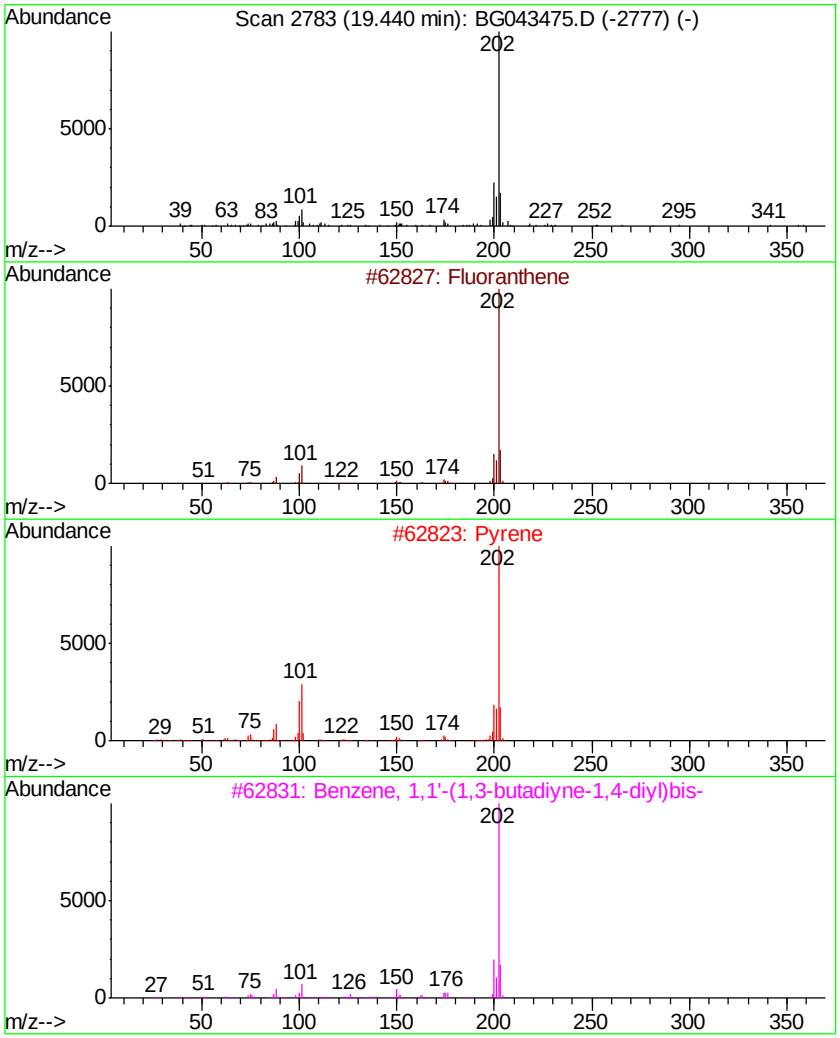
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

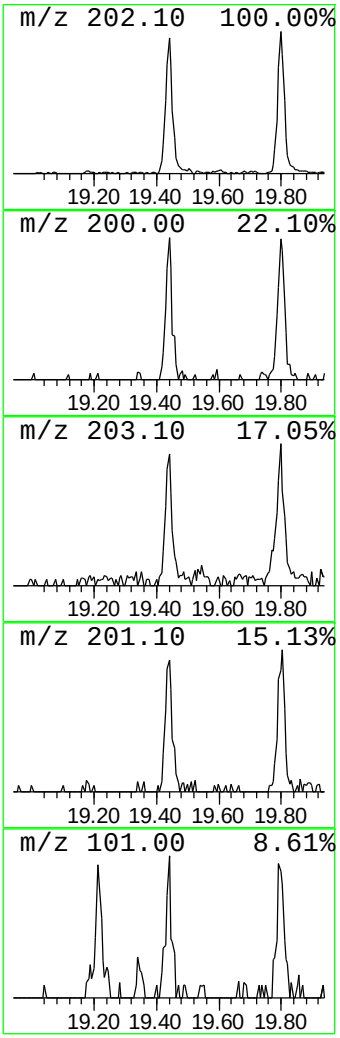
****

Peak Number 8 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.44	2.18 ng	79818	Phenanthrene-d10	17.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	93
2	Pyrene	202	C16H10	000129-00-0	91
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	72
4	1,4-Pentadiyn-3-one, 1,5-diphenyl-	230	C17H10O	015814-30-9	56
5	4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110119\
Data File : BG043475.D
Acq On : 1 Nov 2019 21:10
Operator : JU
Sample : K5143-05 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NB-08-103019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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-methoxy...	3.19	6.4	ng	105093	1	8.02	327360	20.0
2-Pentanone, 4-hy...	5.12	6.5	ng	107234	1	8.02	327360	20.0
unknown7.55	7.55	41.2	ng	674048	1	8.02	327360	20.0
Tridecanoic acid,...	18.05	2.5	ng	92242	4	17.38	731914	20.0
9,12-Octadecadien...	19.18	7.1	ng	260422	4	17.38	731914	20.0
10-Octadecenoic a...	19.21	11.0	ng	401123	4	17.38	731914	20.0
Benzene, 1,1'-(1,...	19.44	2.2	ng	79818	4	17.38	731914	20.0