LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043363.D
Acq On : 28 Oct 2019 23:26
Operator : JU
Sample : K5539-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 162-36-(0-1)

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	13	18	26	rVB	84791	113745	3.23%	0.588%
2	5.127	342	347	356	rBV	53682	84362	2.39%	0.436%
3	5.614	423	430	443	rBV	724158	1242635	35.28%	6.421%
4	7.213	694	702	721	rBV	756236	1442818	40.96%	7.456%
5	7.565	753	762	774	rBV	777749	1389266	39.44%	7.179%
6	8.023	833	840	848	rBV	150994	261547	7.42%	1.352%
7	8.347	886	895	905	rBV	566760	1027682	29.17%	5.311%
8	9.187	1030	1038	1057	rBV	400895	833054	23.65%	4.305%
9	10.832	1310	1318	1328	rBV	153172	323655	9.19%	1.672%
10	13.276	1727	1734	1760	rBV	1190692	1974377	56.05%	10.203%
11	14.099	1869	1874	1888	rBV	66316	131757	3.74%	0.681%
12	14.651	1961	1968	1977	rBV2	306205	528414	15.00%	2.731%
13	16.137	2213	2221	2242	rBV	1168068	2024808	57.48%	10.463%
14	16.960	2354	2361	2373	rBV3	19107	41541	1.18%	0.215%
15	17.395	2428	2435	2440	rBV	422088	675406	19.17%	3.490%
16	17.436	2440	2442	2451	rVV	86595	134152	3.81%	0.693%
17	17.518	2451	2456	2464	rVB6	21655	53972	1.53%	0.279%
18	18.282	2580	2586	2591	rBV4	48401	83730	2.38%	0.433%
19	19.445	2778	2784	2791	rBV	131061	200236	5.68%	1.035%
20	19.810	2836	2846	2855	rBV	107104	216162	6.14%	1.117%
21	20.003	2872	2879	2895	rBV	2555620	3522684	100.00%	18.204%
22	21.308	3096	3101	3113	rBV9	40474	126294	3.59%	0.653%
23	21.660	3149	3161	3167	rBV	515343	1028603	29.20%	5.315%
24	21.848	3189	3193	3201	rVB4	45261	74116	2.10%	0.383%
25	22.448	3291	3295	3302	rVB3	52992	81249	2.31%	0.420%
26	23.135	3405	3412	3422	rVB2	58335	117507	3.34%	0.607%
27	23.329	3439	3445	3451	rVB2	57659	109440	3.11%	0.566%
28	23.852	3526	3534	3541	rBV3	30959	108725	3.09%	0.562%
29	23.934	3541	3548	3555	rVB4	52624	134573	3.82%	0.695%
30	24.563	3649	3655	3660	rBV4	17744	39857	1.13%	0.206%
31	24.704	3671	3679	3687	rBV3	31379	83602	2.37%	0.432%
32	24.857	3694	3705	3720	rBV	346041	1030312	29.25%	5.324%
33	25.985	3890	3897	3907	rBV5	23622	68683	1.95%	0.355%
34	27.336	4118	4127	4137	rVB5	12973	42660	1.21%	0.220%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043363.D
Acq On : 28 Oct 2019 23:26
Operator : JU
Sample : K5539-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
162-36-(0-1)

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

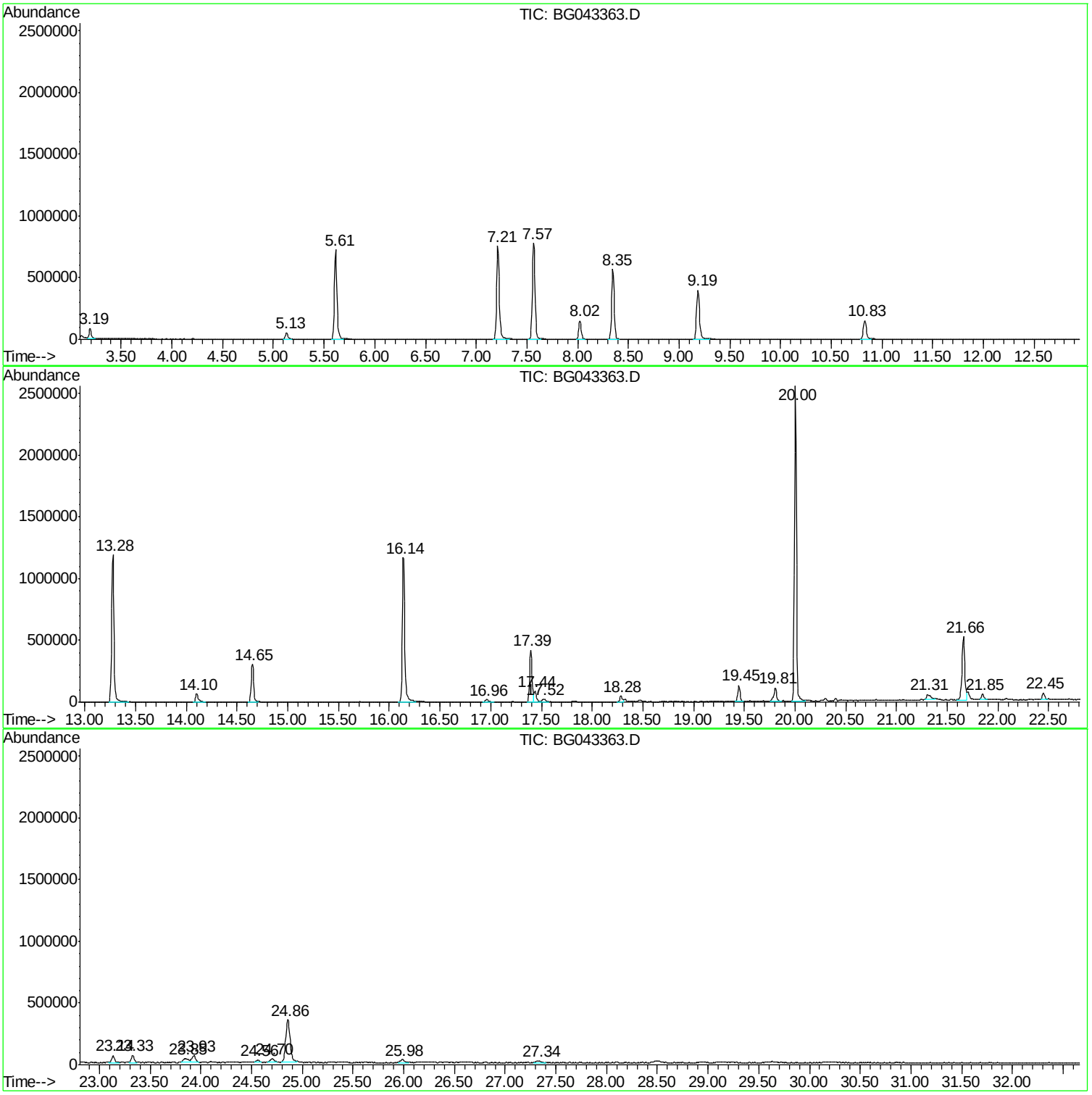
Sum of corrected areas: 19351624

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043363.D
Acq On : 28 Oct 2019 23:26
Operator : JU
Sample : K5539-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
162-36-(0-1)

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\BG102819\
Data File : BG043363.D
Acq On : 28 Oct 2019 23:26
Operator : JU
Sample : K5539-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 162-36-(0-1)

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

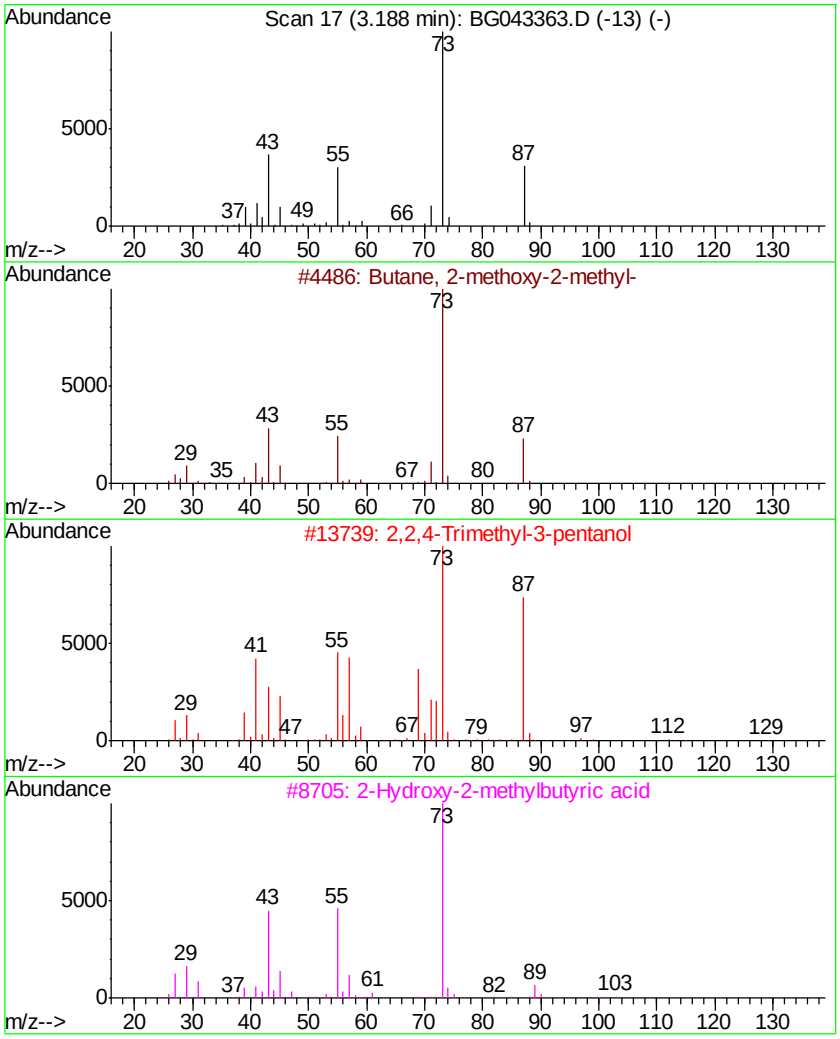
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

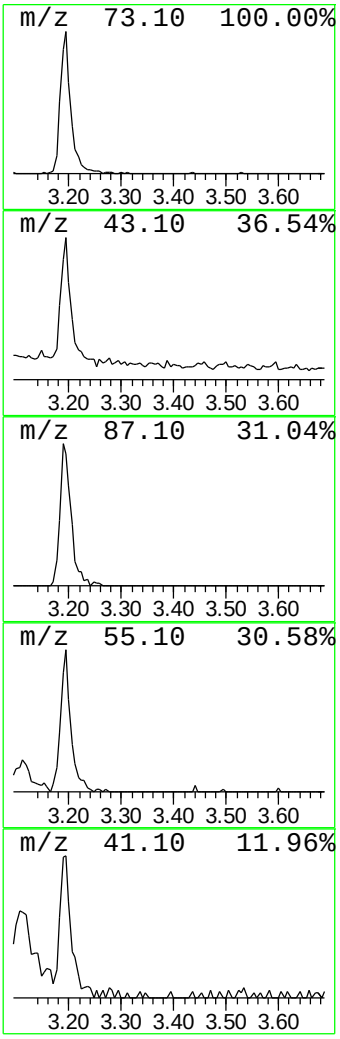
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	8.70 ng	113745	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	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043363.D
Acq On : 28 Oct 2019 23:26
Operator : JU
Sample : K5539-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 162-36-(0-1)

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

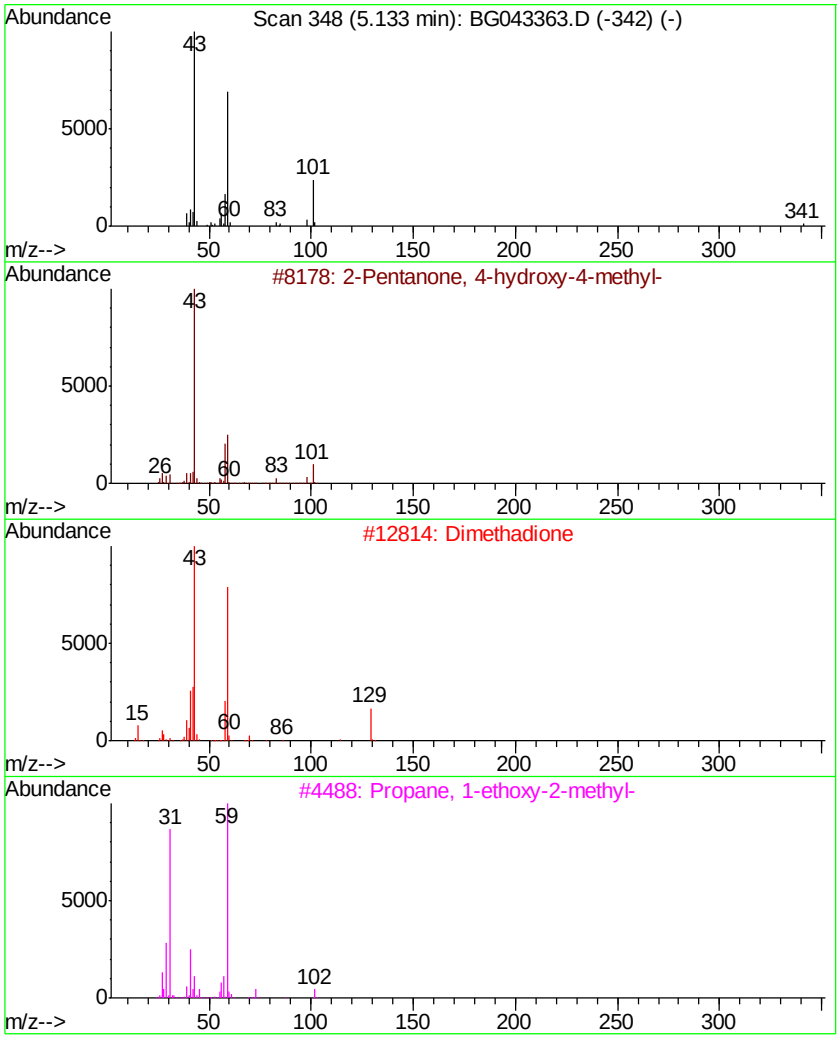
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

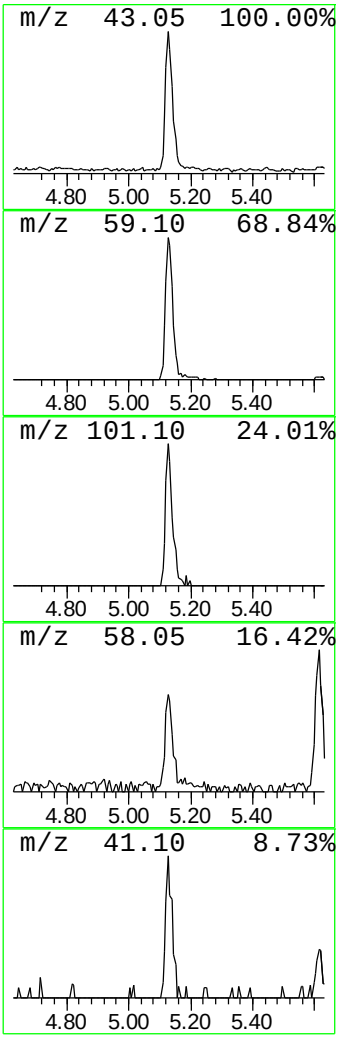
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	6.45 ng	84362	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	64
2	Dimethadione	129	C5H7NO3	000695-53-4	40
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	35
4	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	33
5	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043363.D
Acq On : 28 Oct 2019 23:26
Operator : JU
Sample : K5539-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 162-36-(0-1)

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

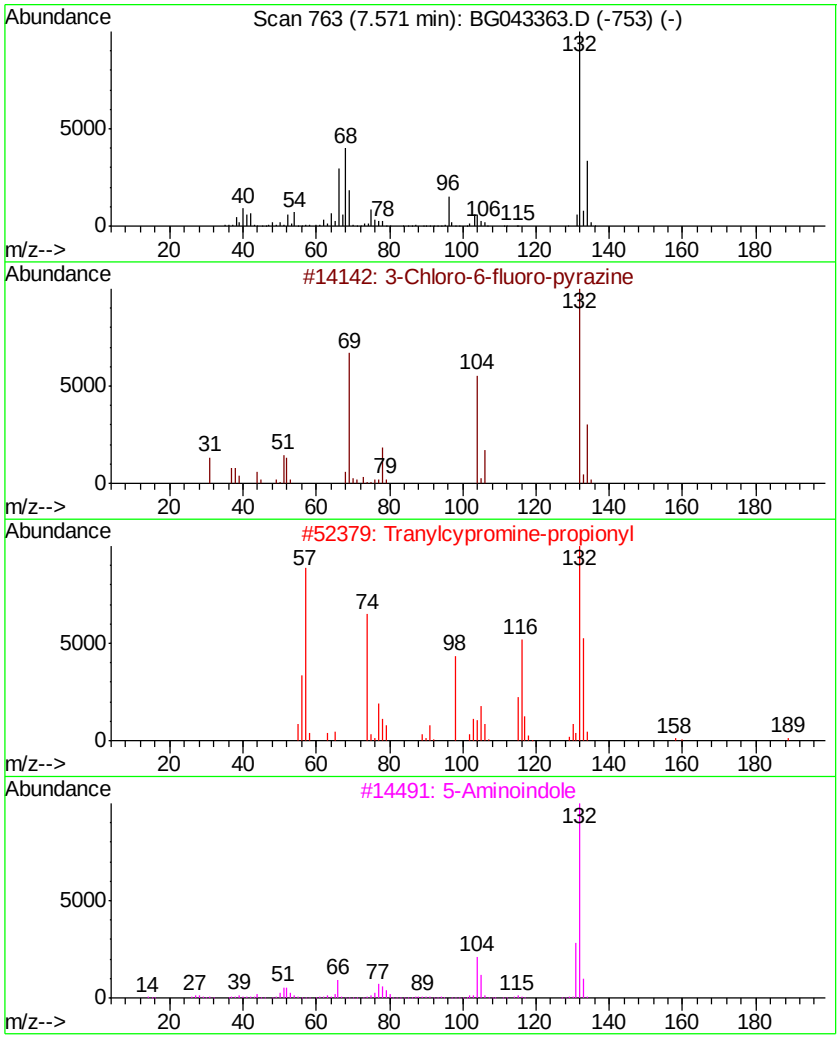
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

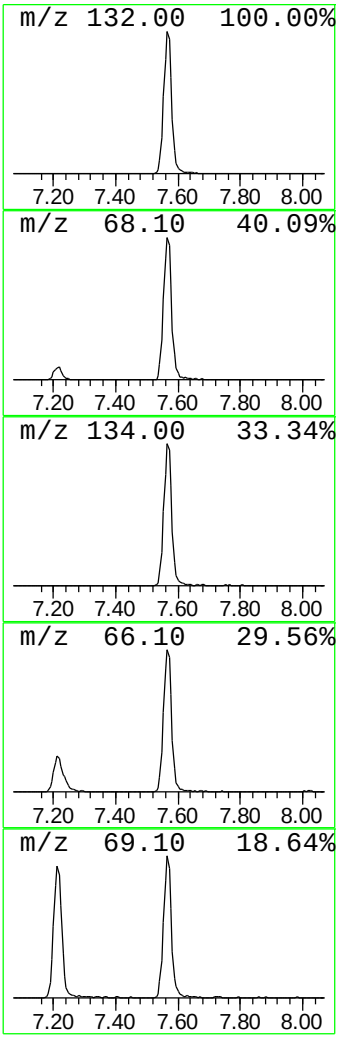
****

Peak Number 3 unknown7.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	106.24 ng	1389270	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	10
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043363.D
Acq On : 28 Oct 2019 23:26
Operator : JU
Sample : K5539-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 162-36-(0-1)

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

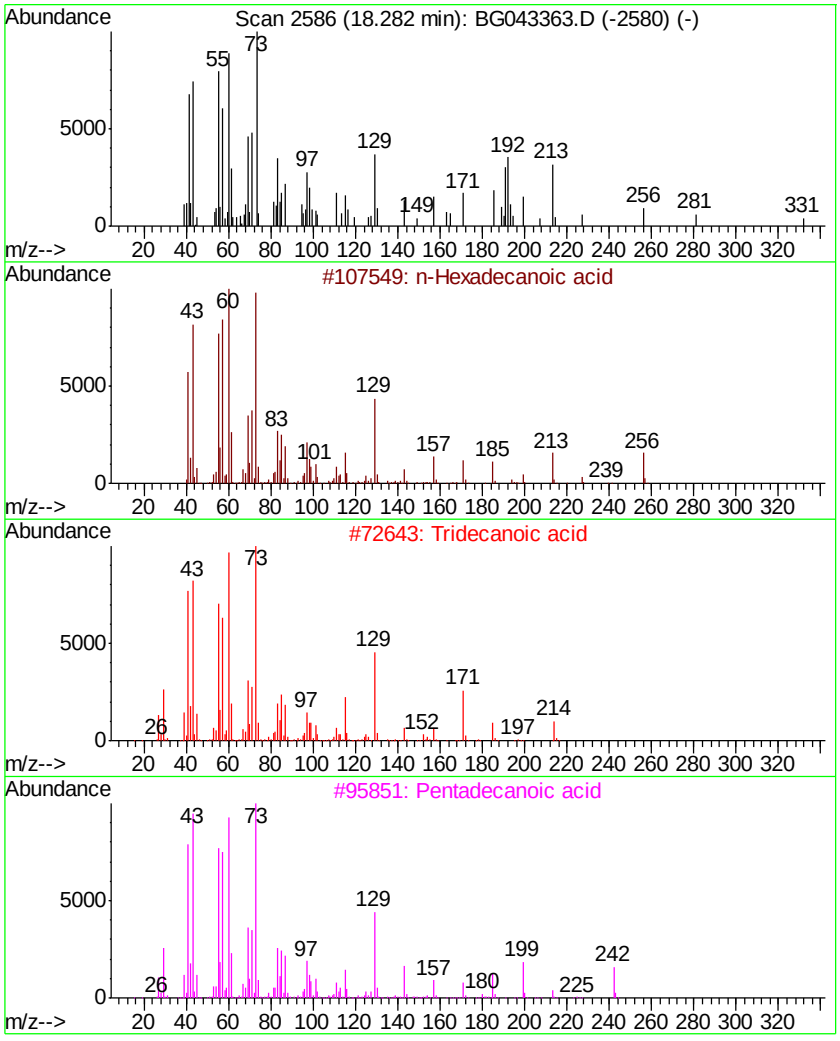
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

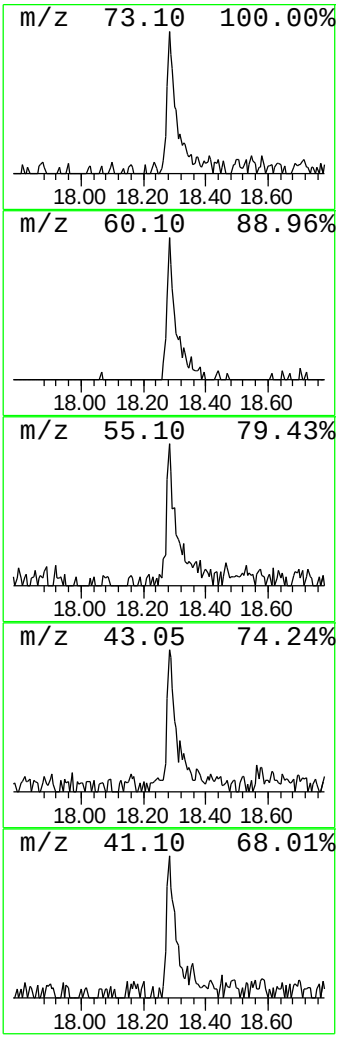
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	2.48 ng	83730	Phenanthrene-d10	17.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	55
2	Tridecanoic acid	214	C13H26O2	000638-53-9	55
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4	Octadecanoic acid	284	C18H36O2	000057-11-4	53
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043363.D
Acq On : 28 Oct 2019 23:26
Operator : JU
Sample : K5539-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 162-36-(0-1)

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

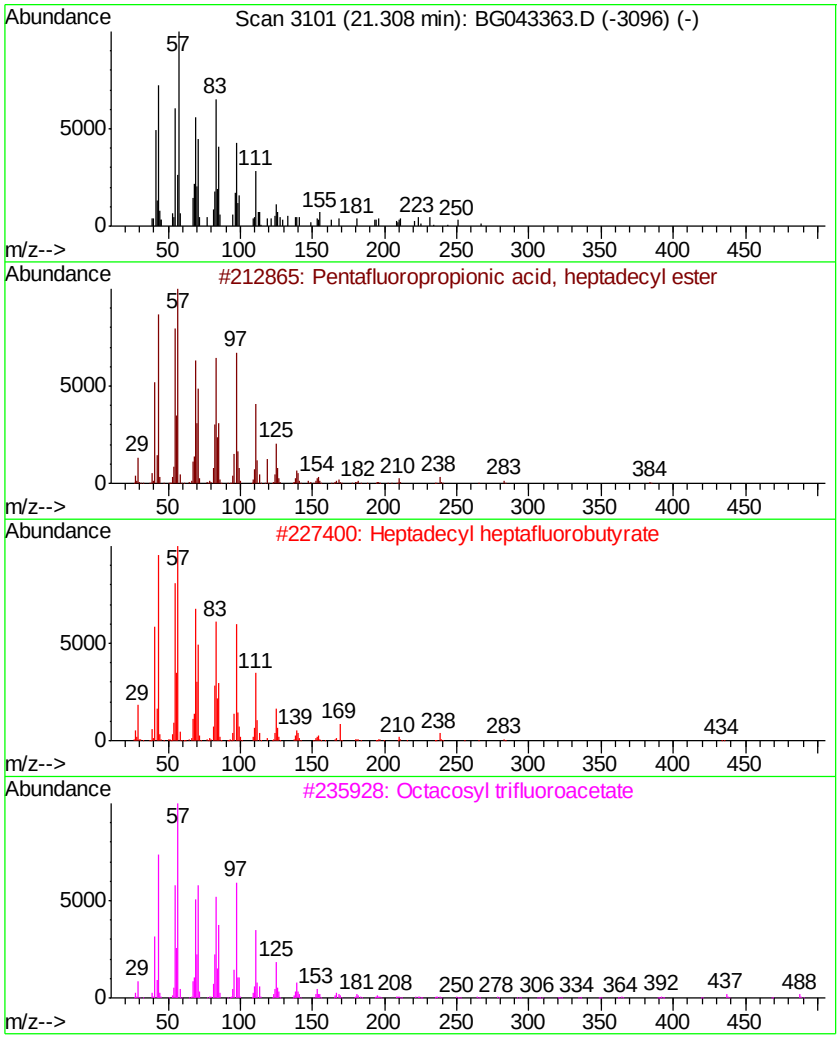
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

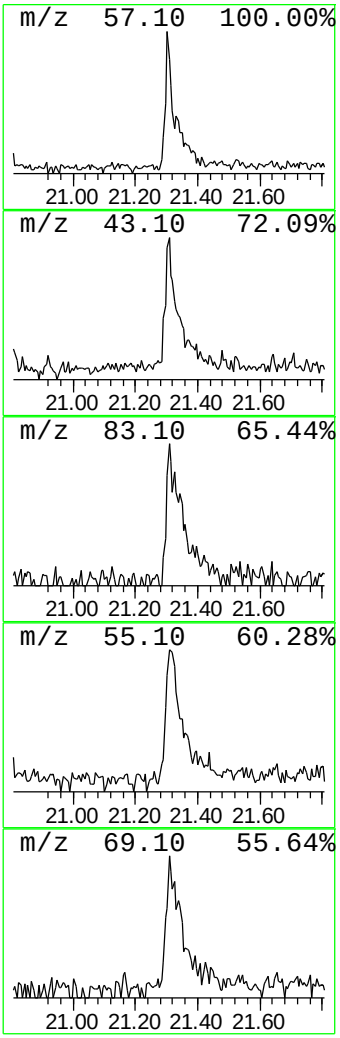
****

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	2.46 ng	126294	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	83
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	81
3	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	76
4	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	74
5	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	74





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043363.D
Acq On : 28 Oct 2019 23:26
Operator : JU
Sample : K5539-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 162-36-(0-1)

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

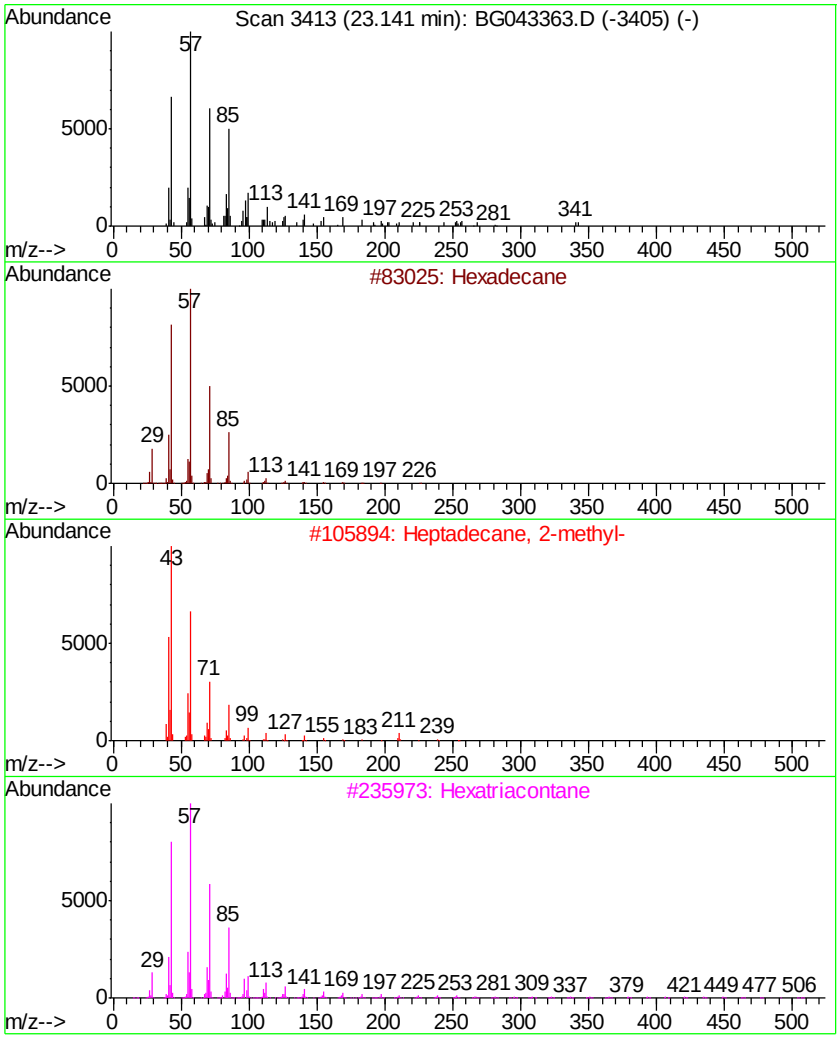
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

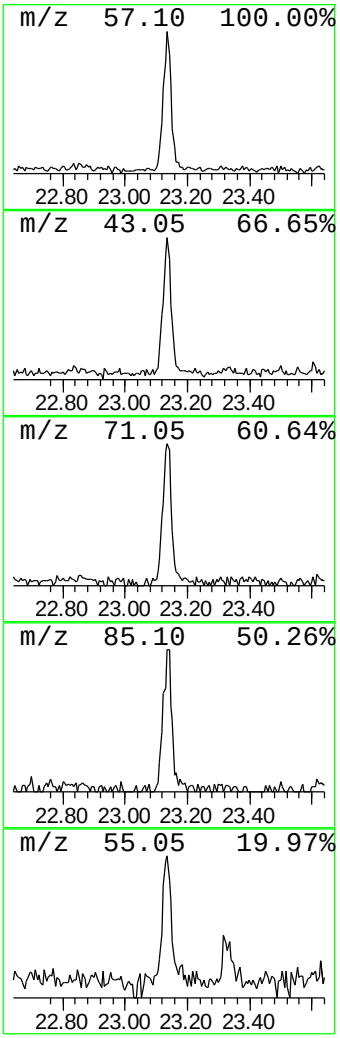
****

Peak Number 7 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.14	2.28 ng	117507	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	94
2	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	93
3	Hexatriacontane	507	C36H74	000630-06-8	90
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	87
5	Heptadecane	240	C17H36	000629-78-7	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043363.D
Acq On : 28 Oct 2019 23:26
Operator : JU
Sample : K5539-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 162-36-(0-1)

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

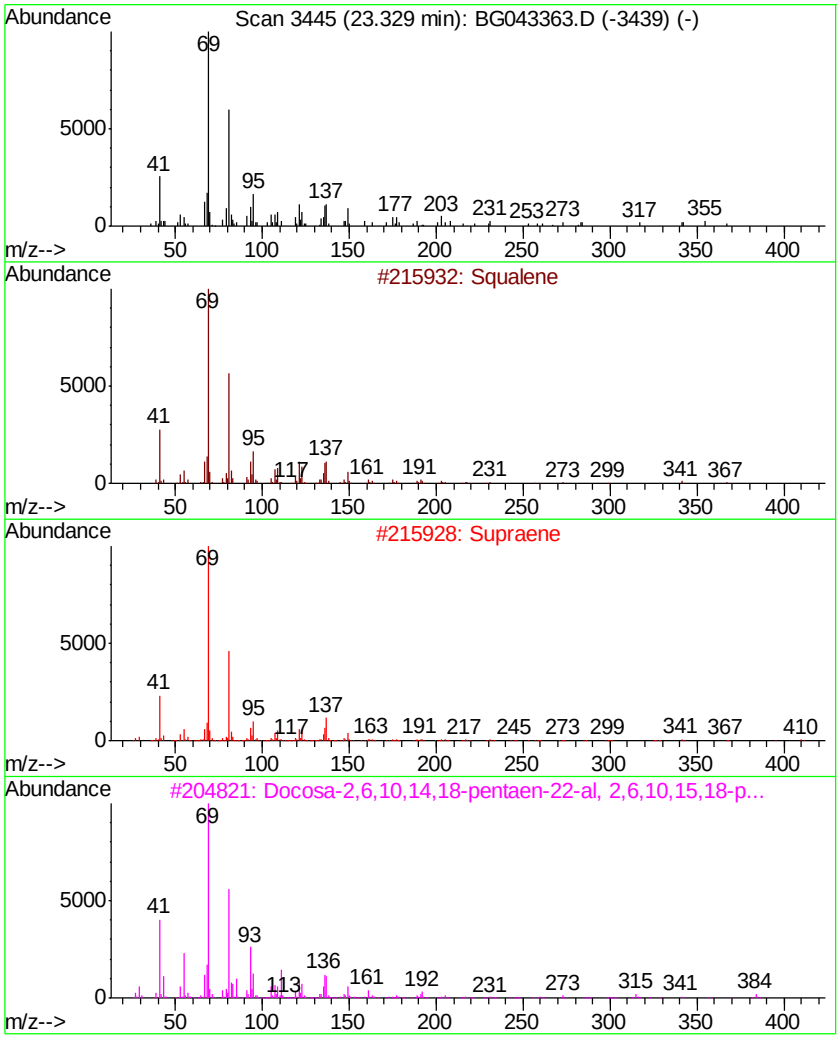
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

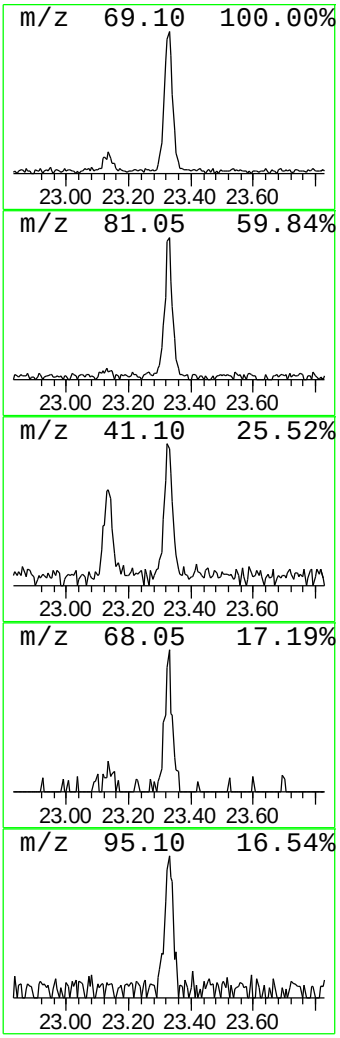
****

Peak Number 8 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.33	2.12 ng	109440	Perylene-d12	24.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	87
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
4	1,6,10,14,18,22-Tetracosahexaen-...	426	C30H50O	054159-46-5	78
5	trans-Farnesol	222	C15H26O	000106-28-5	70





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043363.D
Acq On : 28 Oct 2019 23:26
Operator : JU
Sample : K5539-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 162-36-(0-1)

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

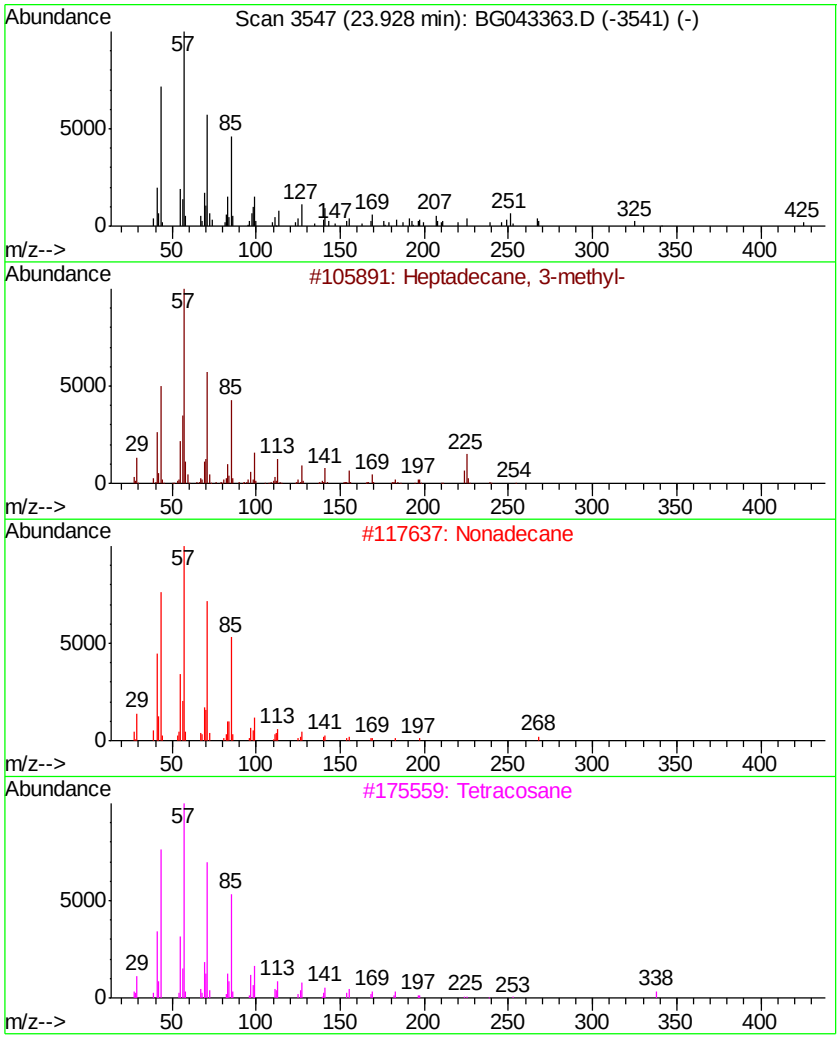
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

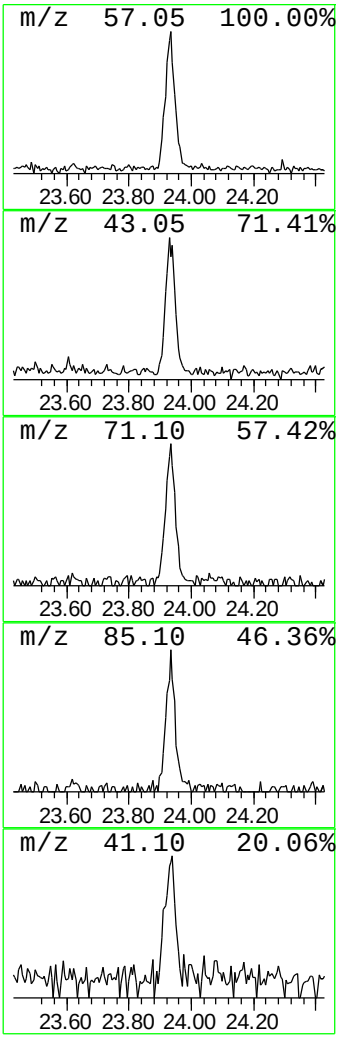
****

Peak Number 9 Heptadecane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.93	2.61 ng	134573	Perylene-d12	24.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 3-methyl-	254	C18H38	006418-44-6	91
2	Nonadecane	268	C19H40	000629-92-5	90
3	Tetracosane	338	C24H50	000646-31-1	80
4	Heptadecane	240	C17H36	000629-78-7	72
5	Decane, 1-iodo-	268	C10H21I	002050-77-3	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG102819\
Data File : BG043363.D
Acq On : 28 Oct 2019 23:26
Operator : JU
Sample : K5539-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
162-36-(0-1)

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	8.7	ng	113745	1	8.02	261547	20.0
2-Pentanone, 4-hy...	5.13	6.5	ng	84362	1	8.02	261547	20.0
unknown7.57	7.57	106.2	ng	1389270	1	8.02	261547	20.0
n-Hexadecanoic acid	18.28	2.5	ng	83730	4	17.39	675406	20.0
Pentafluoropropio...	21.31	2.5	ng	126294	5	21.66	1028600	20.0
Hexadecane	23.14	2.3	ng	117507	5	21.66	1028600	20.0
Squalene	23.33	2.1	ng	109440	6	24.86	1030310	20.0
Heptadecane, 3-me...	23.93	2.6	ng	134573	6	24.86	1030310	20.0