LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
Data File : BG043442.D
Acq On : 31 Oct 2019 20:20
Operator : JU
Sample : K5615-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 3465

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	3.199	13	19	33	rVB	98130	200096	7.82%	1.301%
2	5.132	341	348	358	rBV	114365	191249	7.48%	1.243%
3	5.614	422	430	445	rBV	532592	971458	37.99%	6.316%
4	7.206	693	701	716	rBV	580798	1106048	43.25%	7.191%
5	7.565	753	762	783	rBV	615132	1114751	43.59%	7.247%
6	8.023	833	840	848	rBV	151868	266908	10.44%	1.735%
7	8.346	887	895	908	rBV	450796	819717	32.05%	5.329%
8	9.186	1029	1038	1056	rBV2	306216	643004	25.14%	4.180%
9	10.826	1310	1317	1328	rBV	160954	337080	13.18%	2.191%
10	13.276	1727	1734	1747	rBV	929463	1563892	61.15%	10.167%
11	14.104	1868	1875	1884	rBV	60390	114526	4.48%	0.745%
12	14.651	1961	1968	1983	rBV2	300468	507262	19.84%	3.298%
13	16.137	2214	2221	2240	rBV	798037	1418555	55.47%	9.222%
14	17.394	2427	2435	2452	rBV	371903	639968	25.03%	4.161%
15	17.518	2452	2456	2464	rVB6	13237	25795	1.01%	0.168%
16	18.282	2582	2586	2601	rBV3	74098	145126	5.67%	0.944%
17	19.445	2779	2784	2789	rBV	20248	34894	1.36%	0.227%
18	19.809	2842	2846	2851	rVB3	21214	32232	1.26%	0.210%
19	20.003	2873	2879	2896	rBV	1836569	2557290	100.00%	16.626%
20	20.479	2956	2960	2965	rBV5	19988	32878	1.29%	0.214%
21	20.649	2981	2989	2993	rBV	92880	137692	5.38%	0.895%
22	20.696	2993	2997	3003	rVB9	16896	35434	1.39%	0.230%
23	21.307	3096	3101	3111	rBV3	87220	220277	8.61%	1.432%
24	21.660	3154	3161	3168	rBV	438433	801472	31.34%	5.211%
25	21.848	3189	3193	3202	rVB	37676	58321	2.28%	0.379%
26	22.453	3291	3296	3300	rBV2	53571	80651	3.15%	0.524%
27	23.135	3407	3412	3423	rVB	51551	95486	3.73%	0.621%
28	23.329	3441	3445	3452	rVB2	37675	69733	2.73%	0.453%
29	23.934	3542	3548	3556	rVB4	52943	118422	4.63%	0.770%
30	24.862	3695	3706	3720	rBV2	317985	935650	36.59%	6.083%
31	25.984	3889	3897	3907	rBV7	36524	105642	4.13%	0.687%

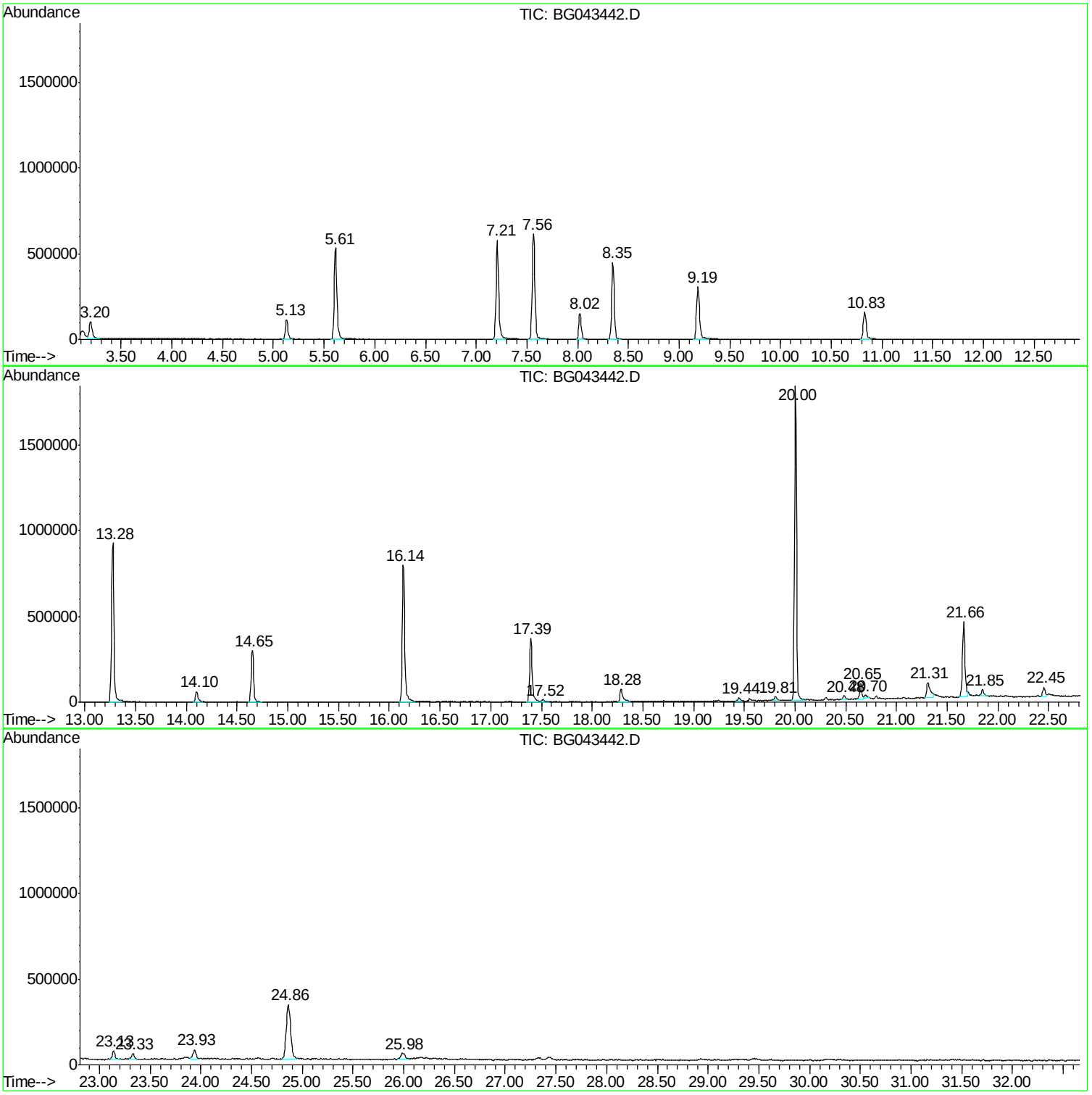
Sum of corrected areas: 15381509

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
Data File : BG043442.D
Acq On : 31 Oct 2019 20:20
Operator : JU
Sample : K5615-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 3465

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



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Data File : BG043442.D
Acq On : 31 Oct 2019 20:20
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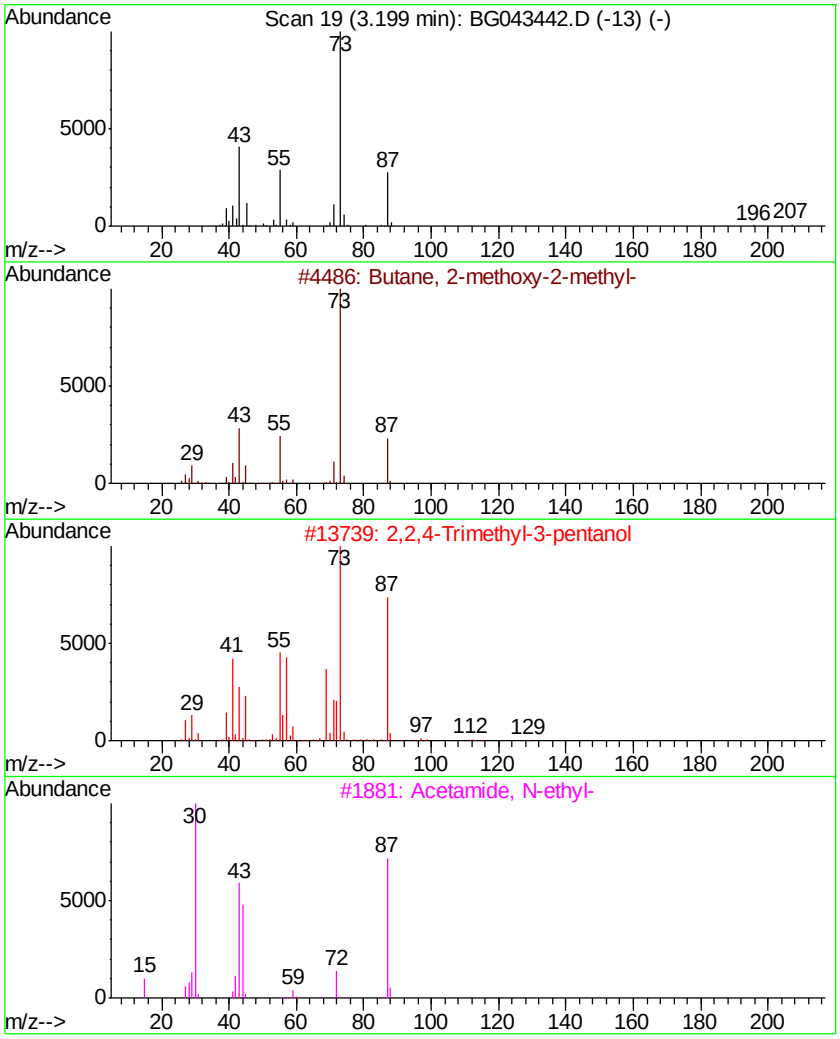
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

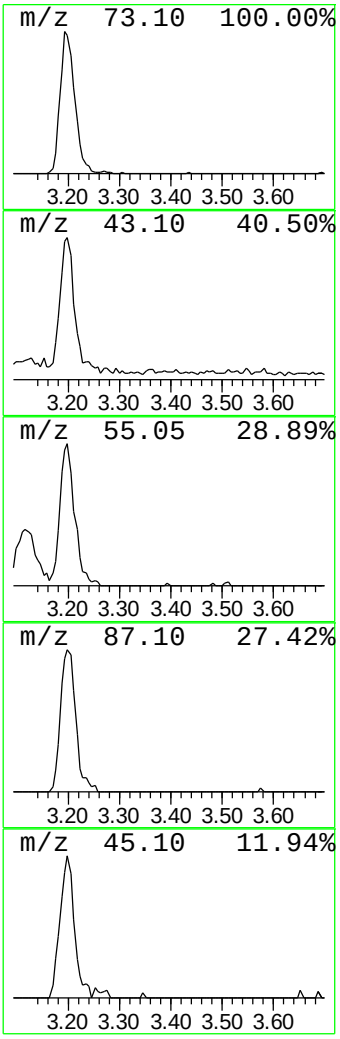
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.20	14.99 ng	200096	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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9





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Data File : BG043442.D
Acq On : 31 Oct 2019 20:20
Operator : JU
Sample : K5615-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 3465

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

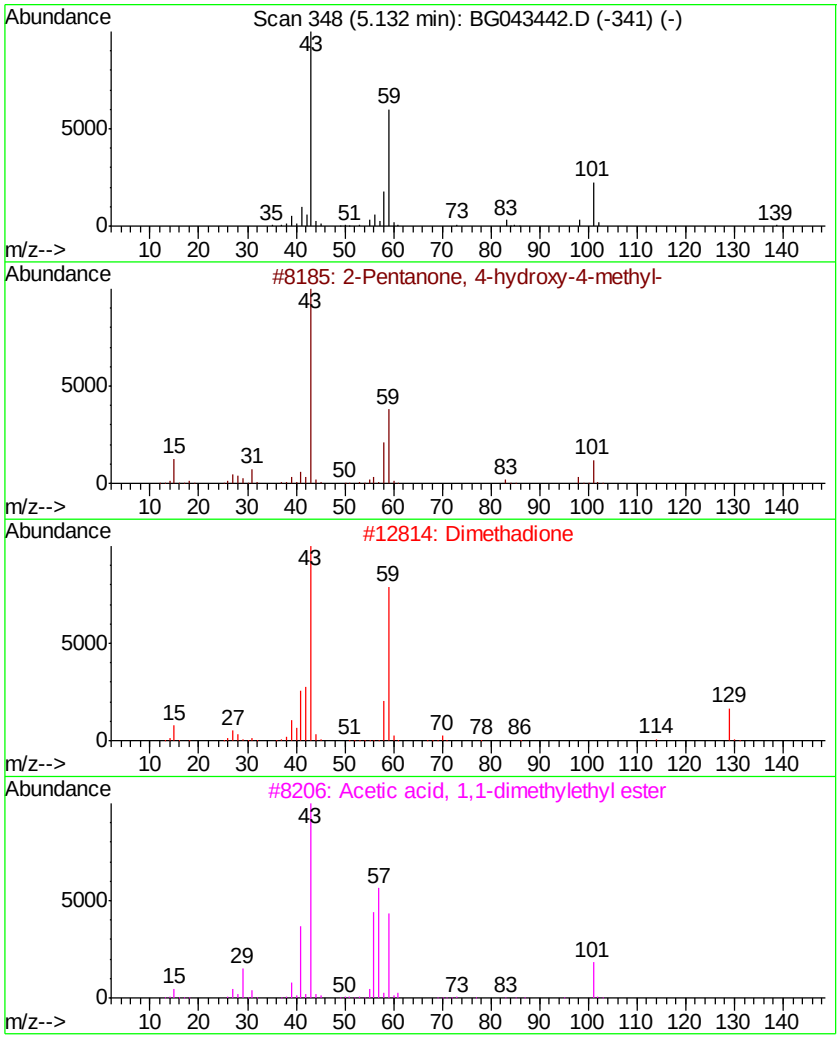
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

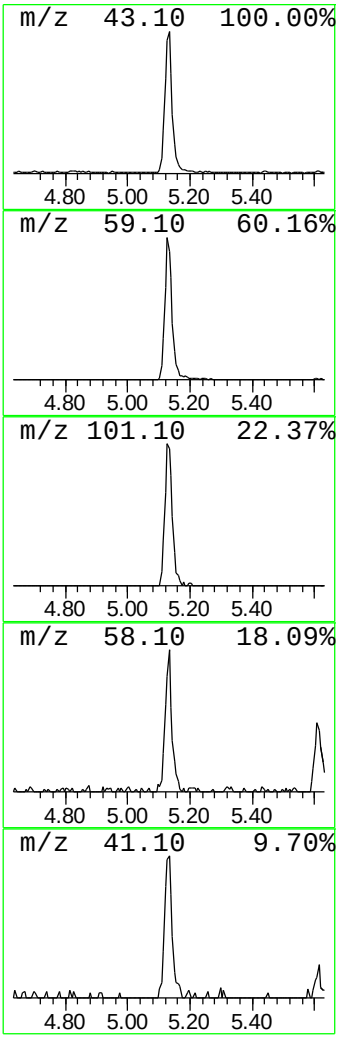
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	14.33 ng	191249	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	56
2	Dimethadione	129	C5H7NO3	000695-53-4	40
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
5	Acetone	58	C3H6O	000067-64-1	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
Data File : BG043442.D
Acq On : 31 Oct 2019 20:20
Operator : JU
Sample : K5615-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 3465

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

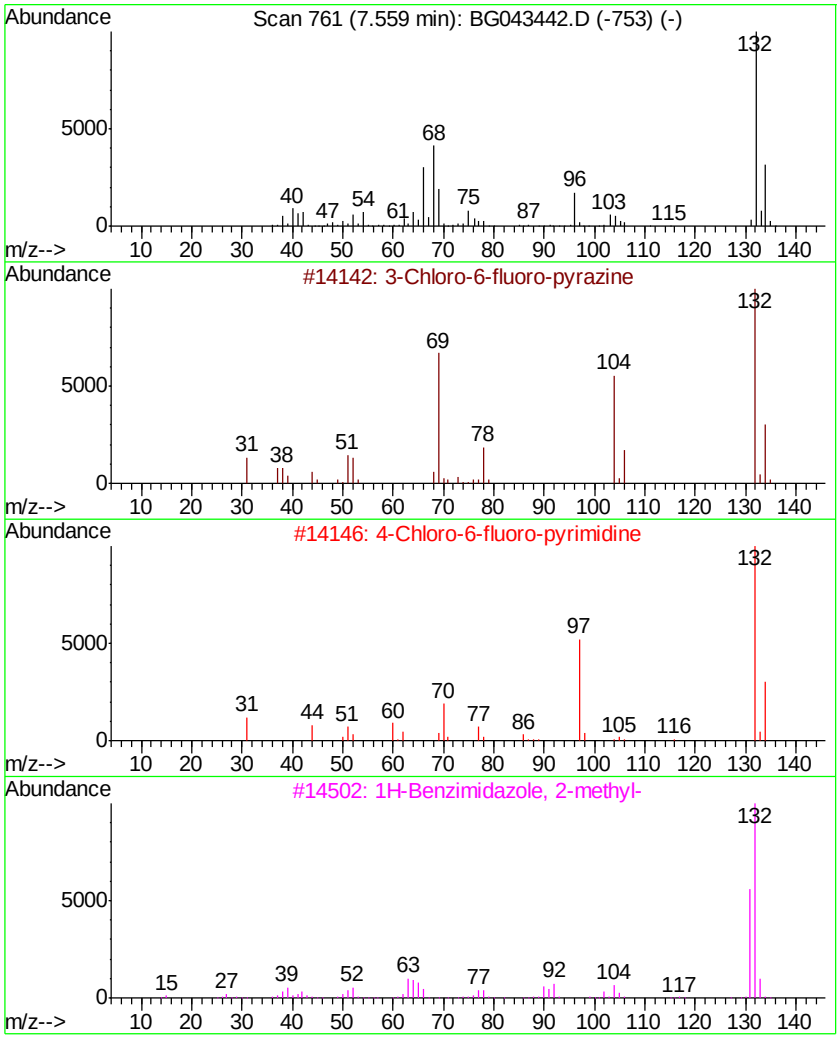
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

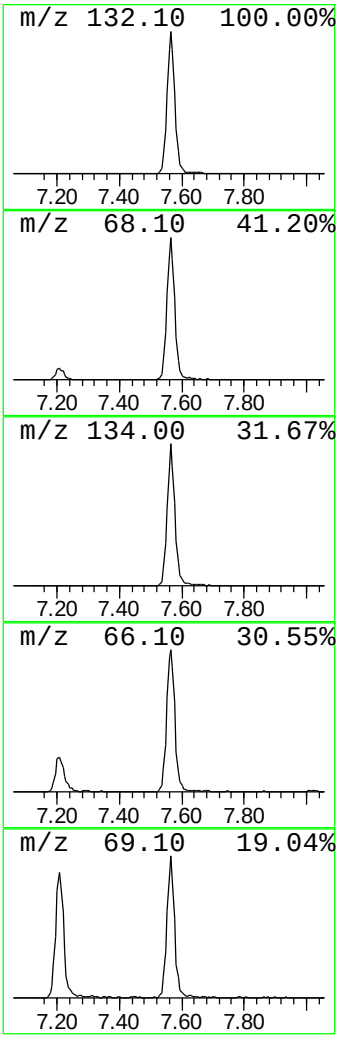
****

Peak Number 3 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	83.53 ng	1114750	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	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
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Operator : JU
Sample : K5615-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 3465

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

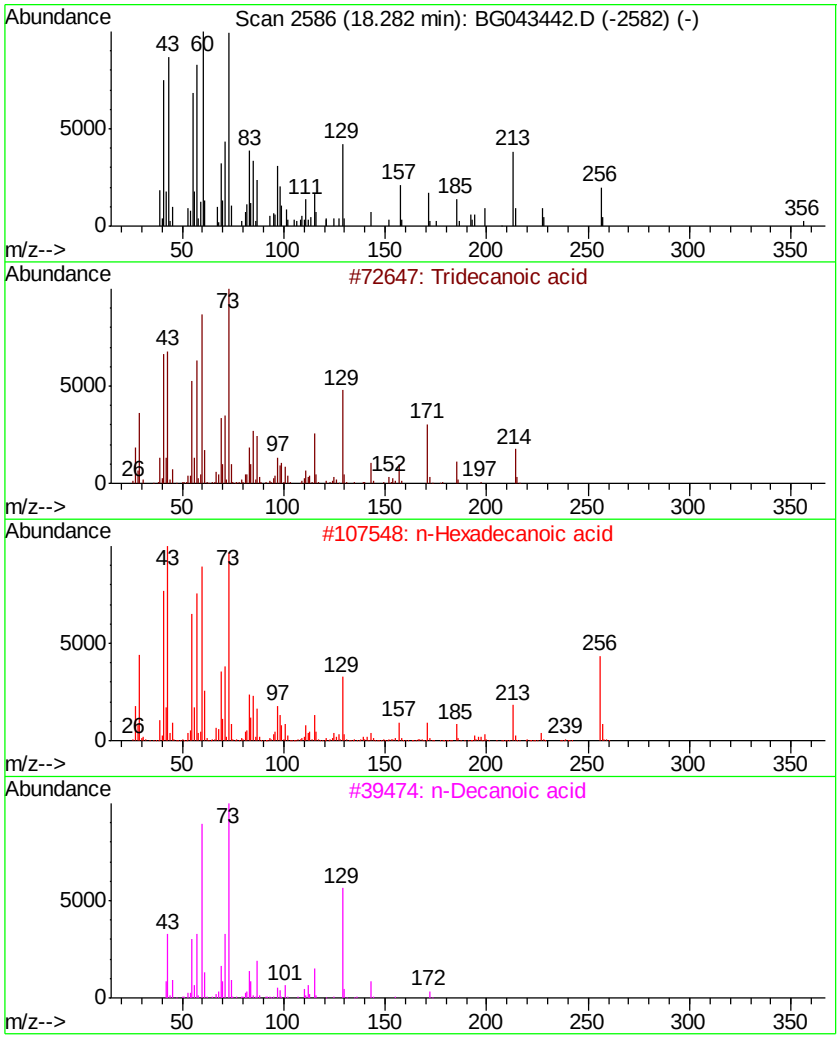
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

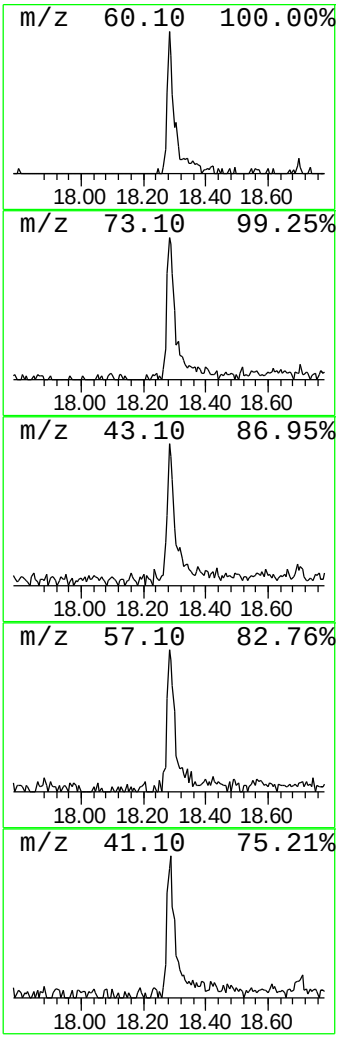
****

Peak Number 5 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	4.54 ng	145126	Phenanthrene-d10	17.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	91
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	n-Decanoic acid	172	C10H20O2	000334-48-5	64
4	Octadecanoic acid	284	C18H36O2	000057-11-4	58
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	55





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
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Operator : JU
Sample : K5615-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 3465

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
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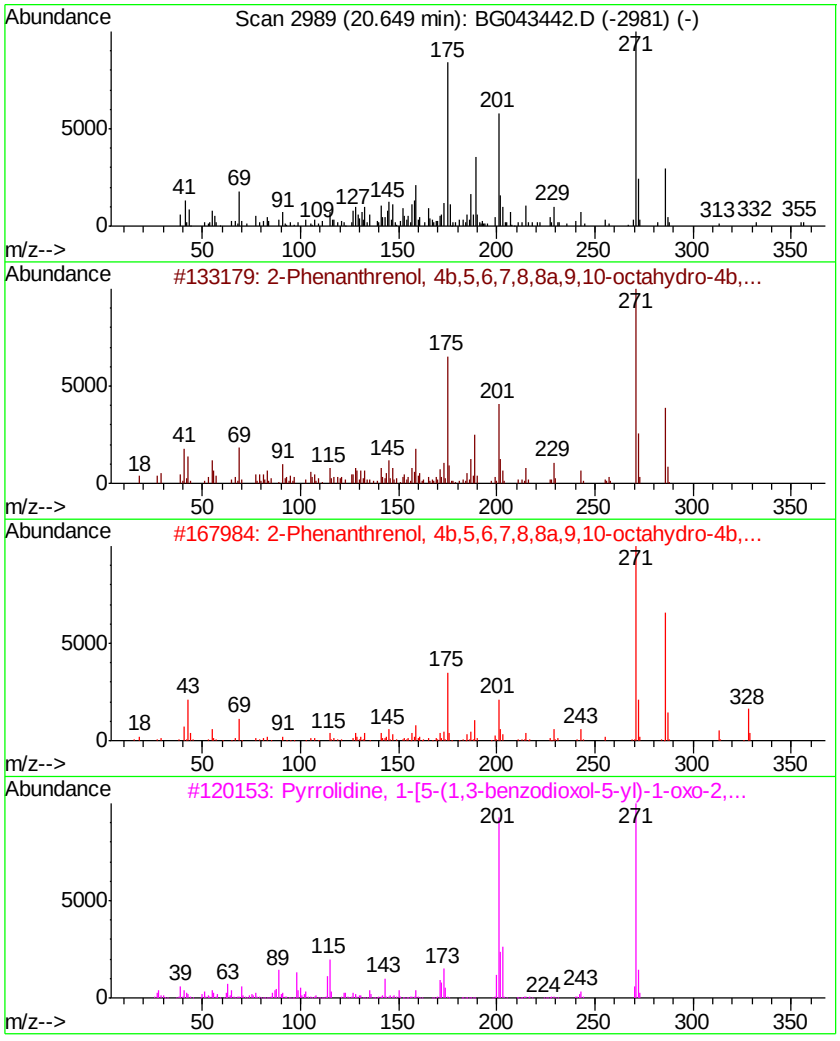
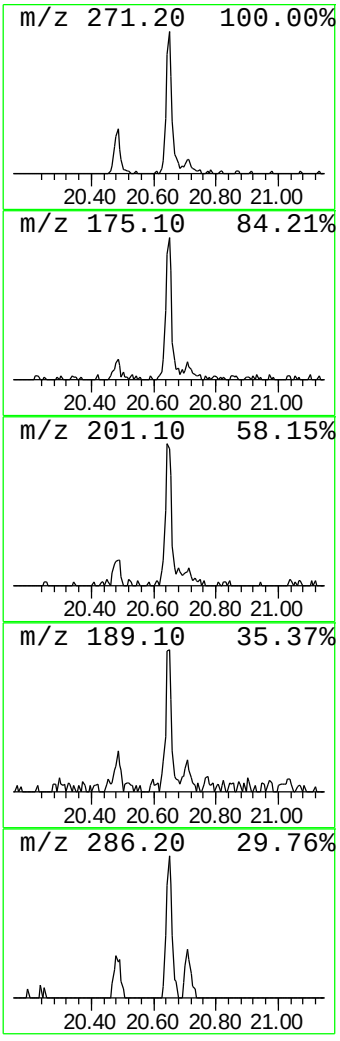
****

Peak Number 6 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.65	3.44 ng	137692	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	95
2	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H32O2	015340-82-6	43
3	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	30
4	Oxazole, 2-(1-naphthalenyl)-5-ph...	271	C19H13NO	000846-63-9	25
5	Dihydronormorphinone	271	C16H17NO3	014696-23-2	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
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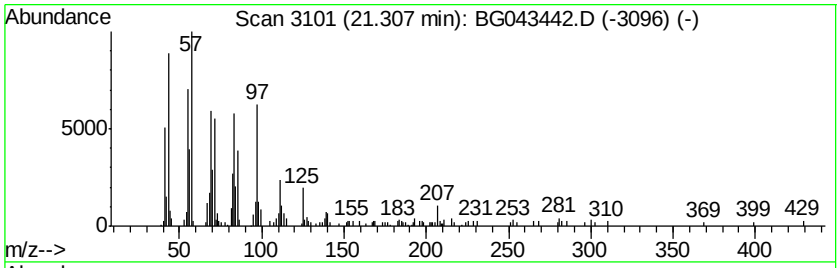
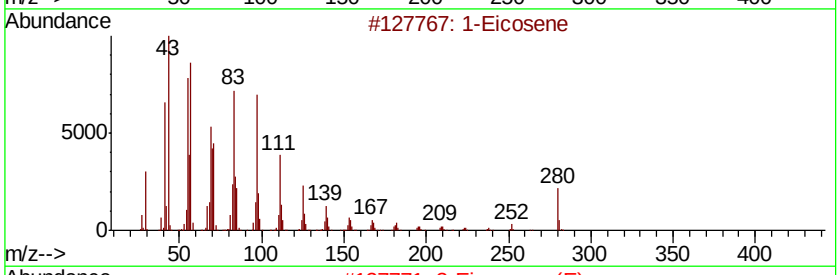
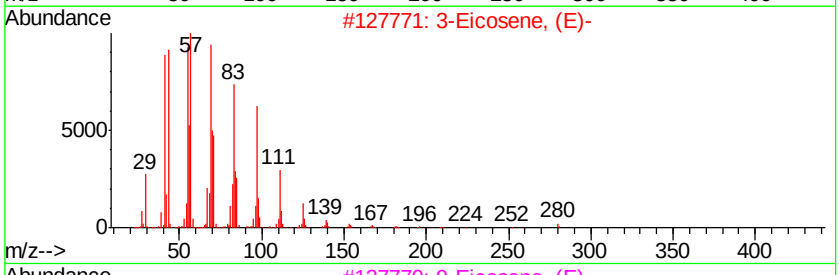
Peak Number 7 1-Eicosene Concentration Rank 5

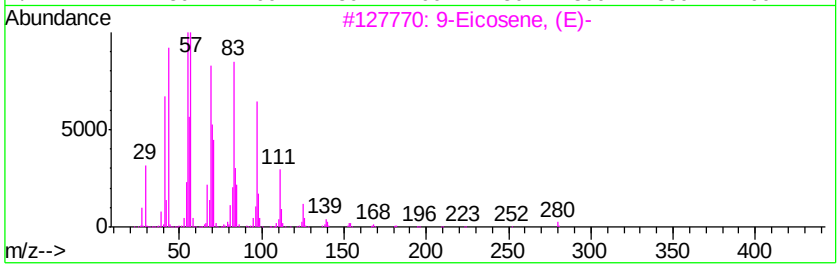
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	5.50 ng	220277	Chrysene-d12	21.66

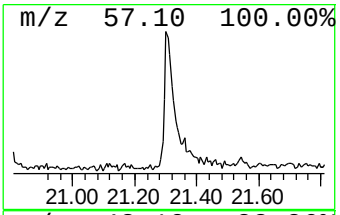
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosene	280	C20H40	003452-07-1	97
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	96
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4	1-Heptacosanol	396	C27H56O	002004-39-9	90
5	Tetracosyl trifluoroacetate	450	C26H49F3O2	1000351-76-4	90

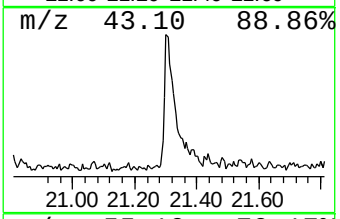


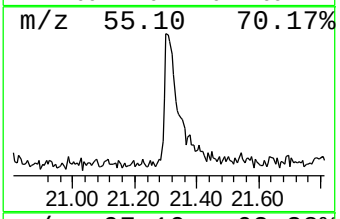


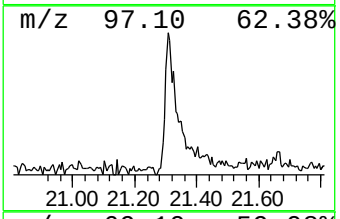


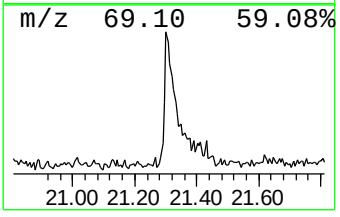












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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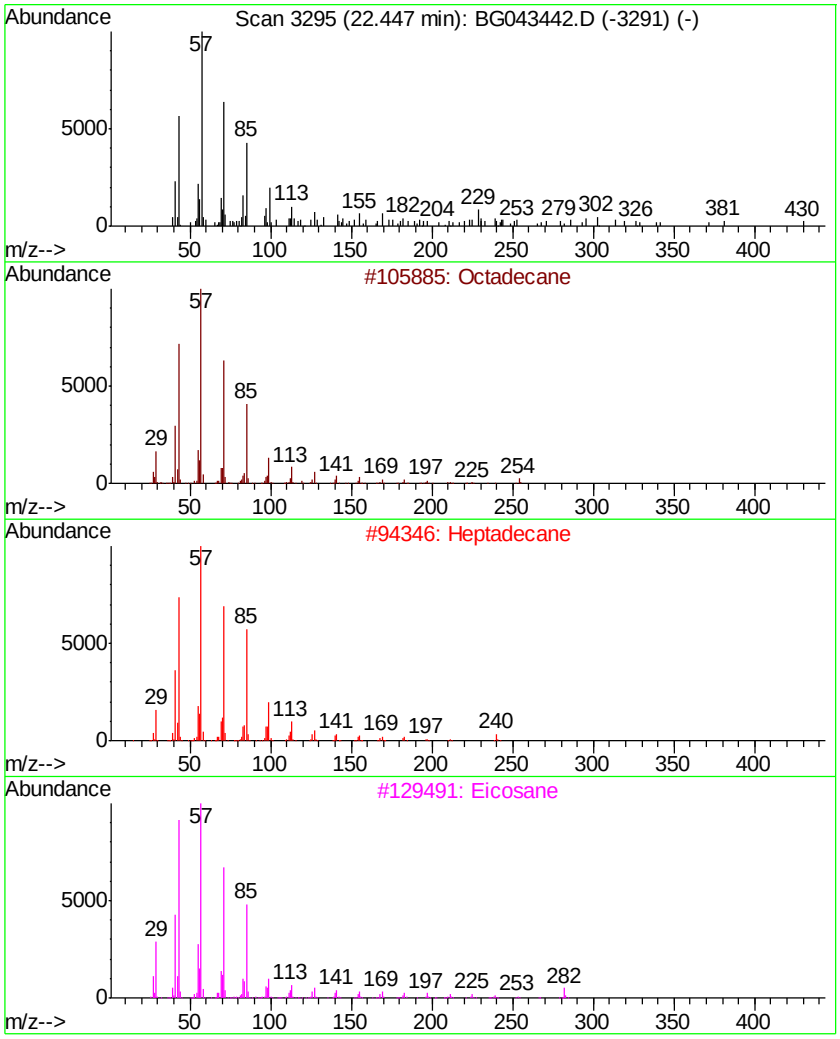
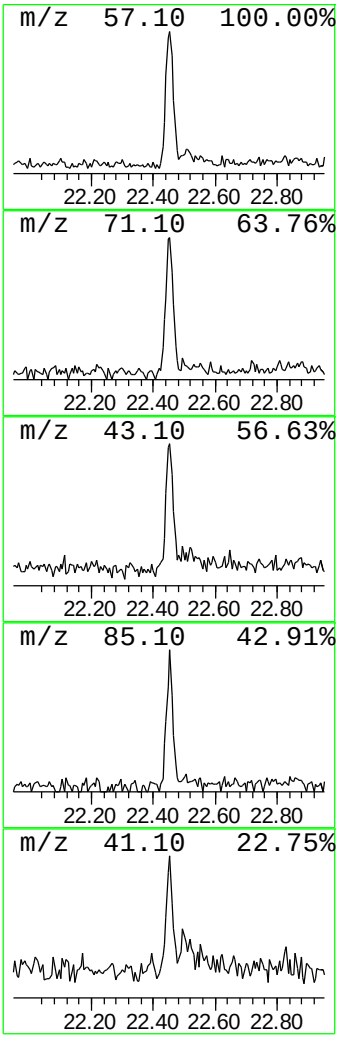
****

Peak Number 8 Octadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.45	2.01 ng	80651	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	95
2	Heptadecane	240	C17H36	000629-78-7	93
3	Eicosane	282	C20H42	000112-95-8	90
4	Pentacosane	352	C25H52	000629-99-2	87
5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	87





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Data File : BG043442.D
Acq On : 31 Oct 2019 20:20
Operator : JU
Sample : K5615-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
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TIC Library : C:\Database\NIST11.L
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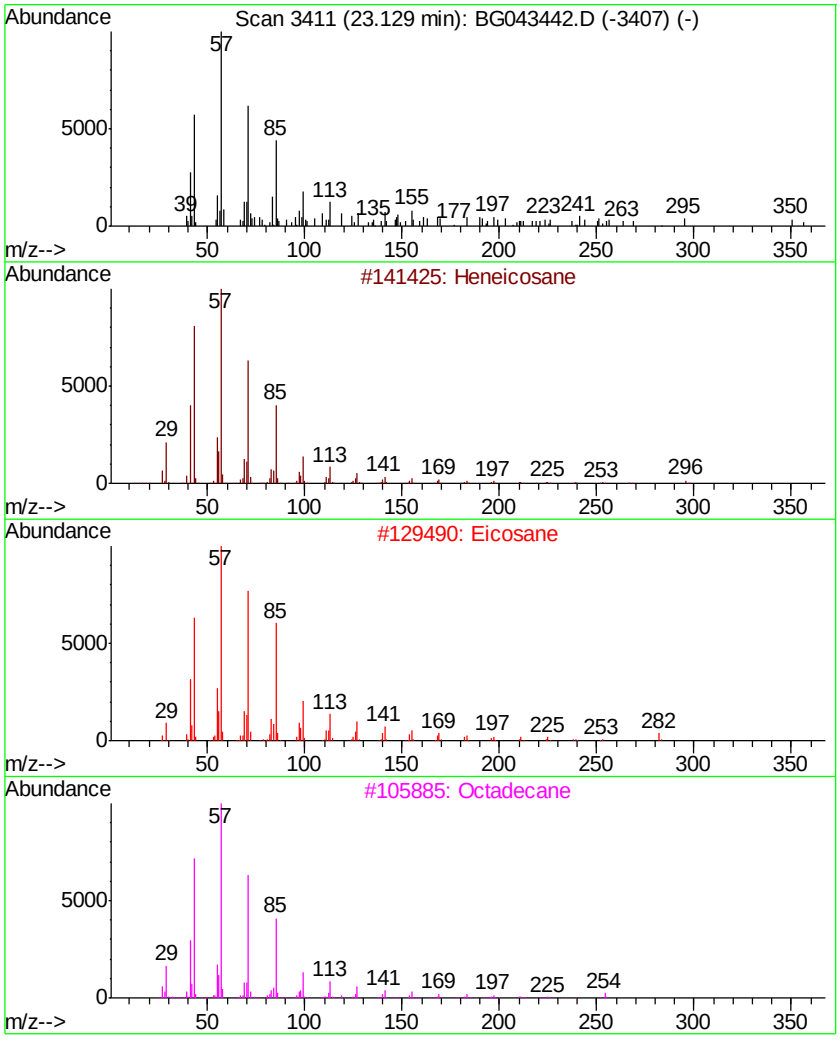
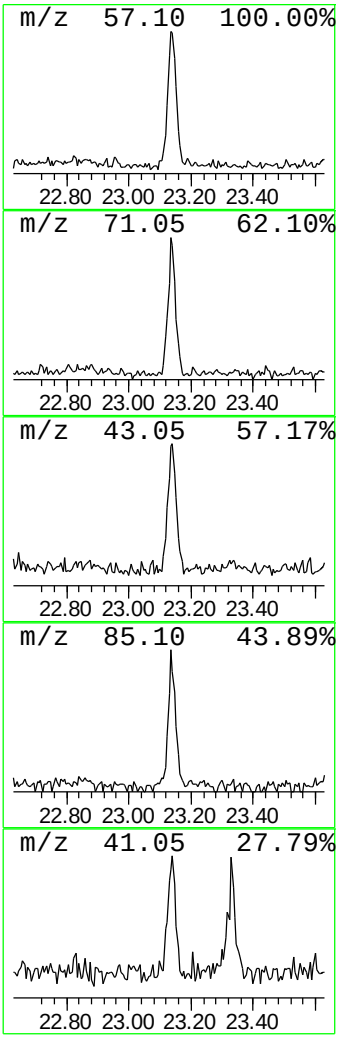
Peak Number 9 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.13	2.38 ng	95486	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	Eicosane	282	C20H42	000112-95-8	95
3	Octadecane	254	C18H38	000593-45-3	94
4	Hexacosane	366	C26H54	000630-01-3	90
5	5,5-Dibutylnonane	240	C17H36	006008-17-9	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
Data File : BG043442.D
Acq On : 31 Oct 2019 20:20
Operator : JU
Sample : K5615-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 3465

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

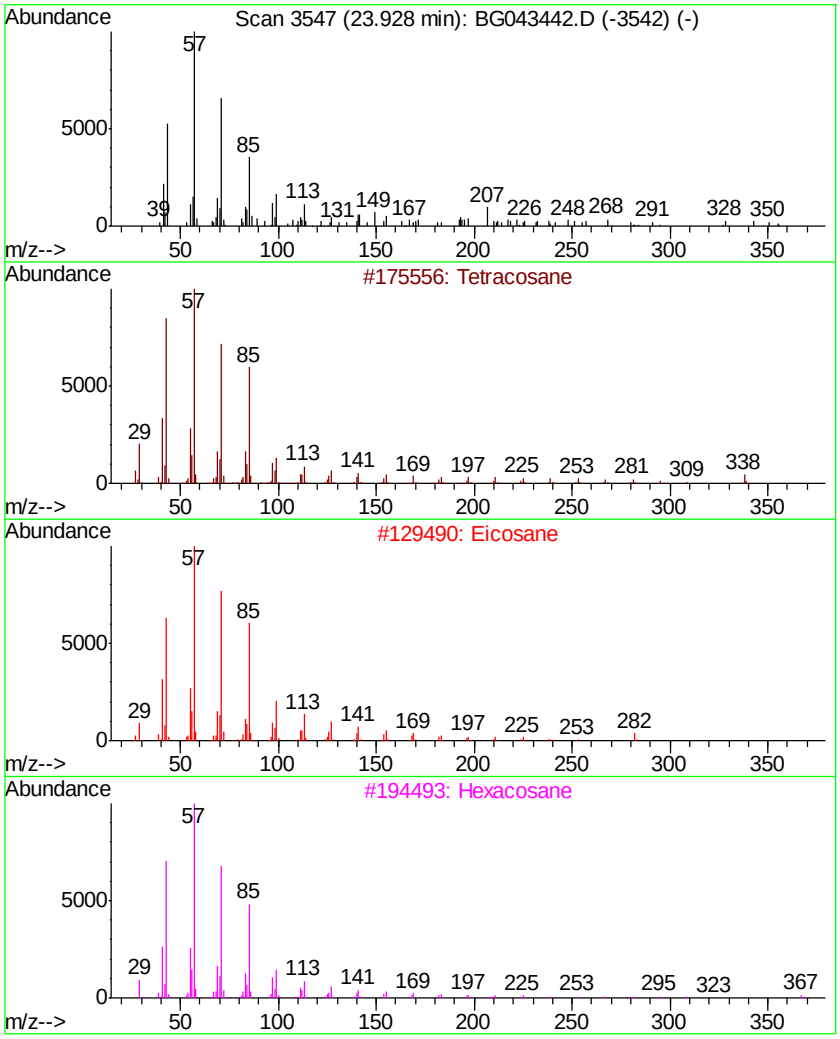
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

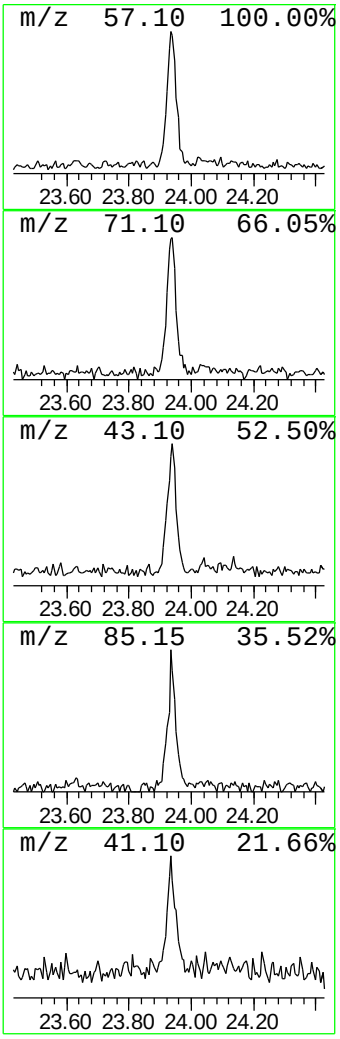
****

Peak Number 10 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.93	2.53 ng	118422	Perylene-d12	24.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Eicosane	282	C20H42	000112-95-8	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Triacontane	422	C30H62	000638-68-6	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
Data File : BG043442.D
Acq On : 31 Oct 2019 20:20
Operator : JU
Sample : K5615-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 3465

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

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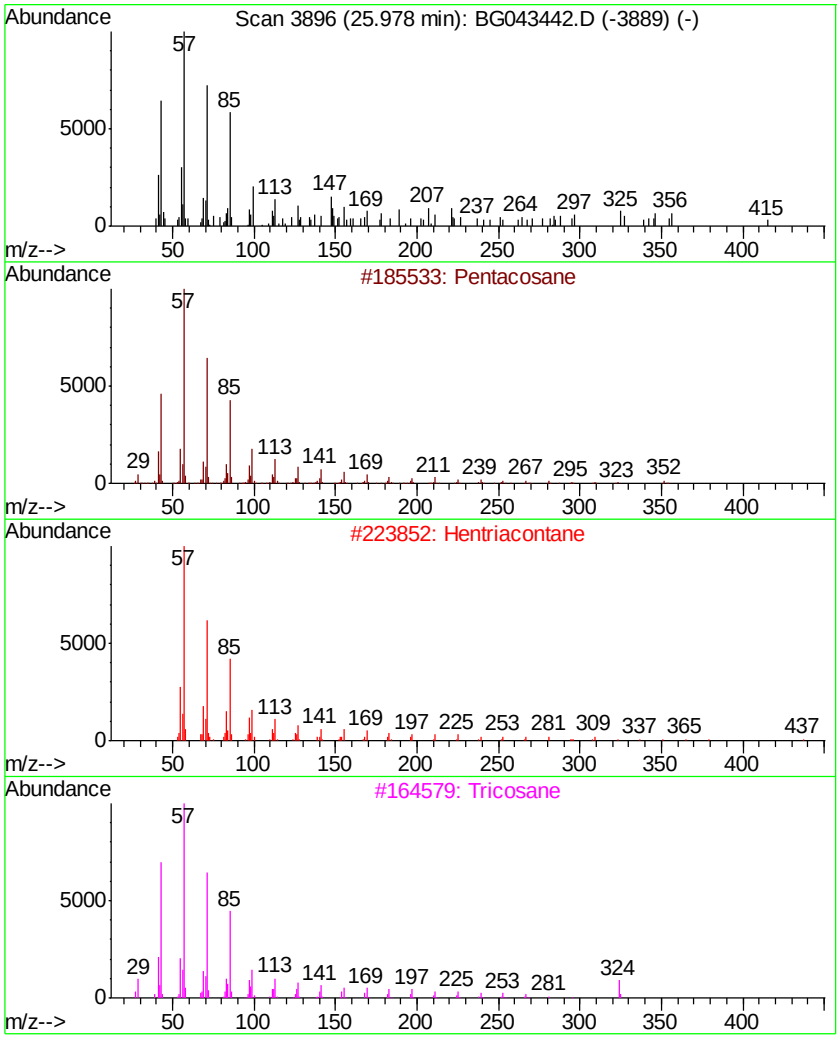
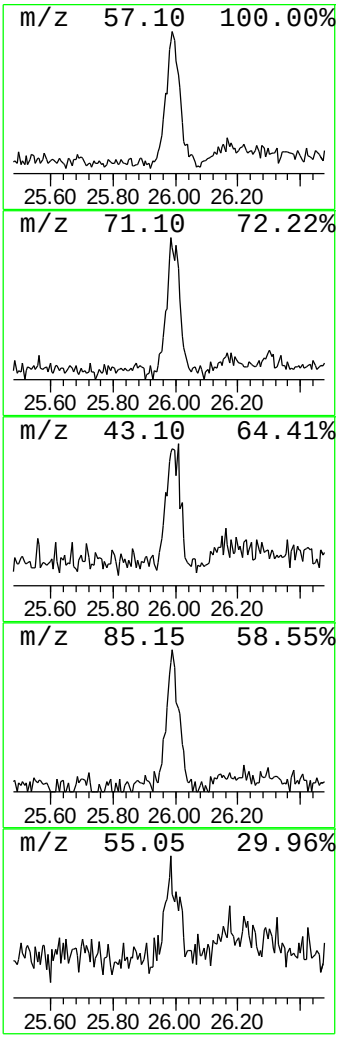
Peak Number 11 Pentacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.98	2.26 ng	105642	Perylene-d12	24.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	62
2	Hentriacontane	437	C31H64	000630-04-6	62
3	Tricosane	324	C23H48	000638-67-5	62
4	Eicosane	282	C20H42	000112-95-8	62
5	Hexadecane	226	C16H34	000544-76-3	60





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG103119\
Data File : BG043442.D
Acq On : 31 Oct 2019 20:20
Operator : JU
Sample : K5615-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 3465

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...	3.20	15.0	ng	200096	1	8.02	266908	20.0
2-Pentanone, 4-hy...	5.13	14.3	ng	191249	1	8.02	266908	20.0
unknown7.56	7.56	83.5	ng	1114750	1	8.02	266908	20.0
Tridecanoic acid	18.28	4.5	ng	145126	4	17.39	639968	20.0
2-Phenanthrenol, ...	20.65	3.4	ng	137692	5	21.66	801472	20.0
1-Eicosene	21.31	5.5	ng	220277	5	21.66	801472	20.0
Octadecane	22.45	2.0	ng	80651	5	21.66	801472	20.0
Heneicosane	23.13	2.4	ng	95486	5	21.66	801472	20.0
Tetracosane	23.93	2.5	ng	118422	6	24.86	935650	20.0
Pentacosane	25.98	2.3	ng	105642	6	24.86	935650	20.0