LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
Data File : BG043448.D
Acq On : 1 Nov 2019 00:13
Operator : JU
Sample : K5620-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-25-S

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	3.200	13	19	29	rVB	90385	182797	7.71%	1.289%
2	5.133	342	348	360	rVB	123960	206614	8.71%	1.457%
3	5.615	421	430	440	rBV	490814	858194	36.18%	6.051%
4	7.213	694	702	714	rBV	535651	1031394	43.48%	7.272%
5	7.565	755	762	772	rBV	568834	1012138	42.67%	7.136%
6	8.024	833	840	849	rBV	152862	275159	11.60%	1.940%
7	8.347	888	895	908	rBV	413519	751374	31.67%	5.297%
8	9.187	1027	1038	1056	rBV	298663	620501	26.16%	4.375%
9	10.832	1309	1318	1327	rBV	171399	350662	14.78%	2.472%
10	13.276	1724	1734	1744	rBV	907653	1510872	63.69%	10.652%
11	14.099	1867	1874	1890	rBV	121266	215616	9.09%	1.520%
12	14.651	1960	1968	1982	rBV	322616	540684	22.79%	3.812%
13	16.138	2214	2221	2235	rBV	643633	1181638	49.81%	8.331%
14	17.395	2429	2435	2450	rBV	400258	652408	27.50%	4.600%
15	20.004	2873	2879	2892	rBV	1781322	2372220	100.00%	16.725%
16	21.308	3095	3101	3109	rBV3	59968	131385	5.54%	0.926%
17	21.660	3155	3161	3173	rBV2	415093	797935	33.64%	5.626%
18	21.849	3188	3193	3199	rBV4	28438	47131	1.99%	0.332%
19	22.454	3290	3296	3300	rBV	44773	68033	2.87%	0.480%
20	23.141	3397	3413	3419	rBV5	58831	175043	7.38%	1.234%
21	23.329	3439	3445	3453	rBV	58096	114323	4.82%	0.806%
22	23.934	3542	3548	3554	rVB3	44941	93598	3.95%	0.660%
23	24.863	3696	3706	3718	rBV	306032	918835	38.73%	6.478%
24	25.997	3890	3899	3908	rVB8	24368	75060	3.16%	0.529%

Sum of corrected areas: 14183614

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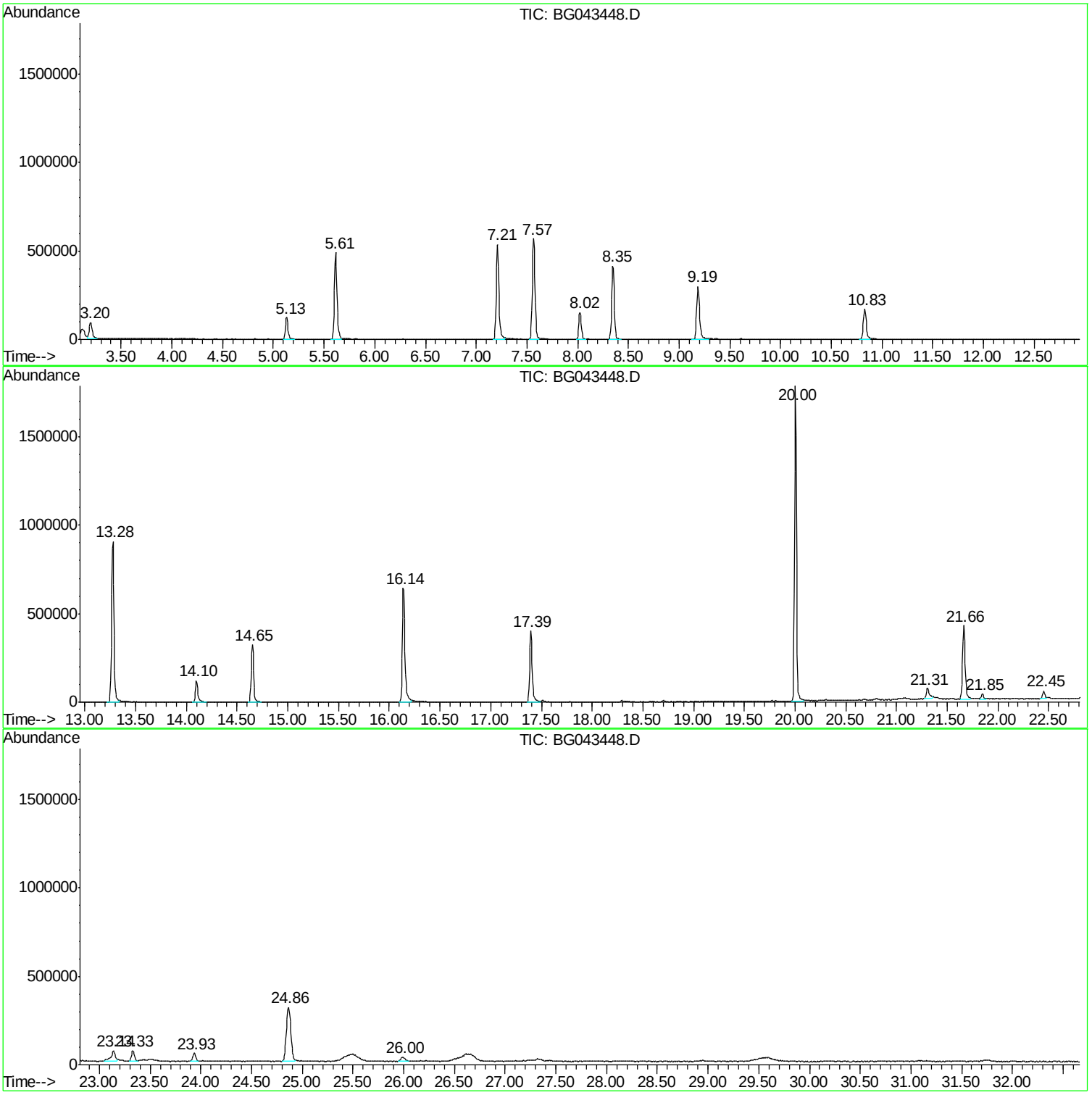
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-25-S

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
Data File : BG043448.D
Acq On : 1 Nov 2019 00:13
Operator : JU
Sample : K5620-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-25-S

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

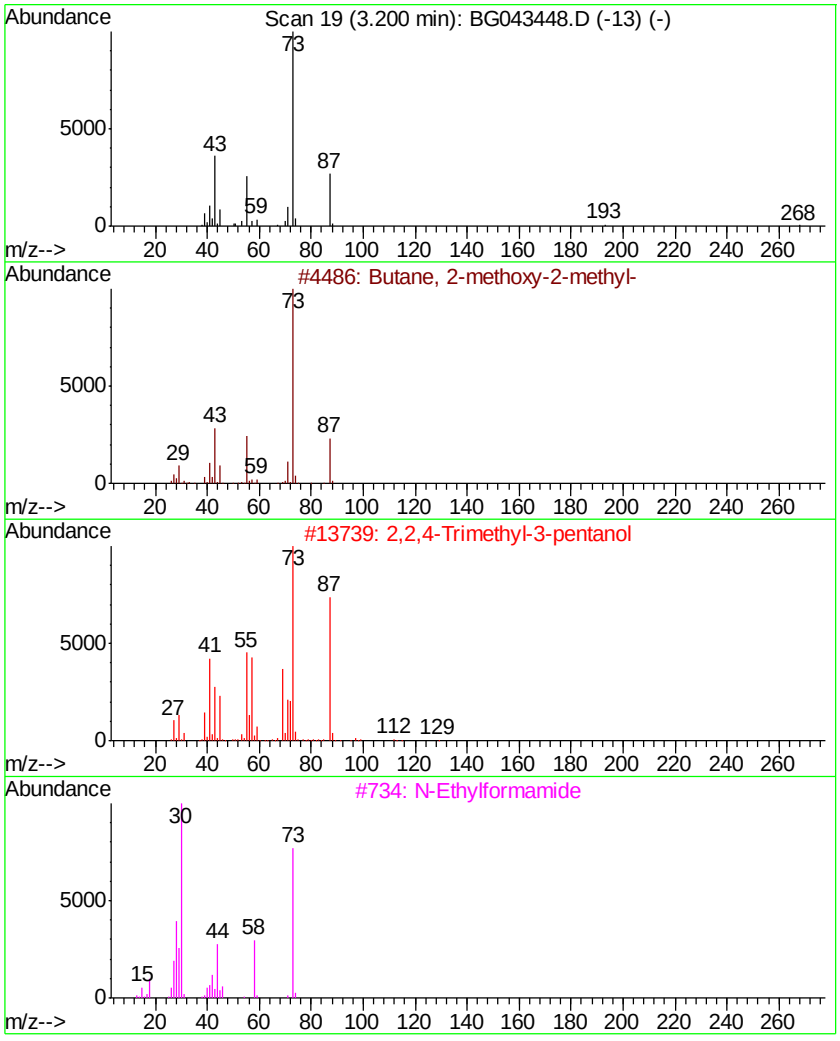
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

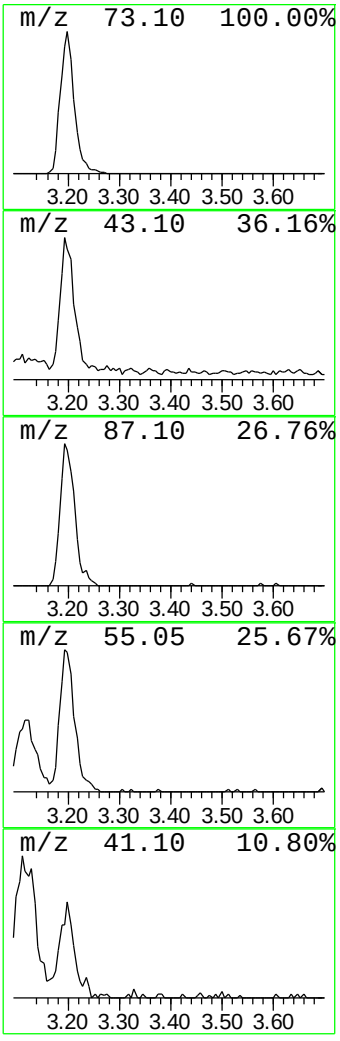
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.20	13.29 ng	182797	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	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9
5	4-Hydroxybutyric acid hydrazide	118	C4H10N2O2	003879-08-1	9





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Acq On : 1 Nov 2019 00:13
Operator : JU
Sample : K5620-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-25-S

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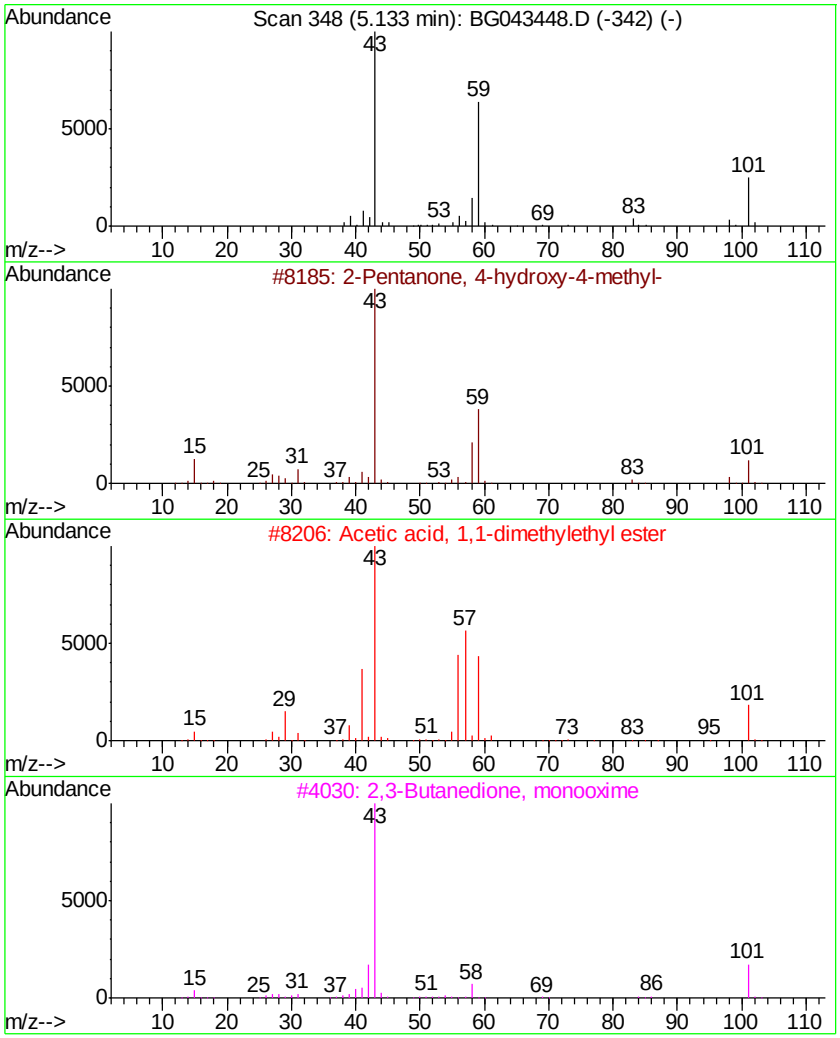
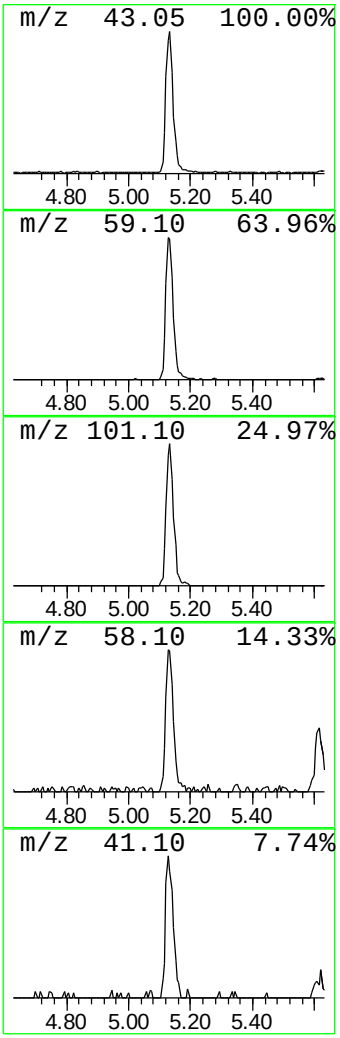
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	15.02 ng	206614	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	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	3-Pentanol	88	C5H12O	000584-02-1	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
Data File : BG043448.D
Acq On : 1 Nov 2019 00:13
Operator : JU
Sample : K5620-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-25-S

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

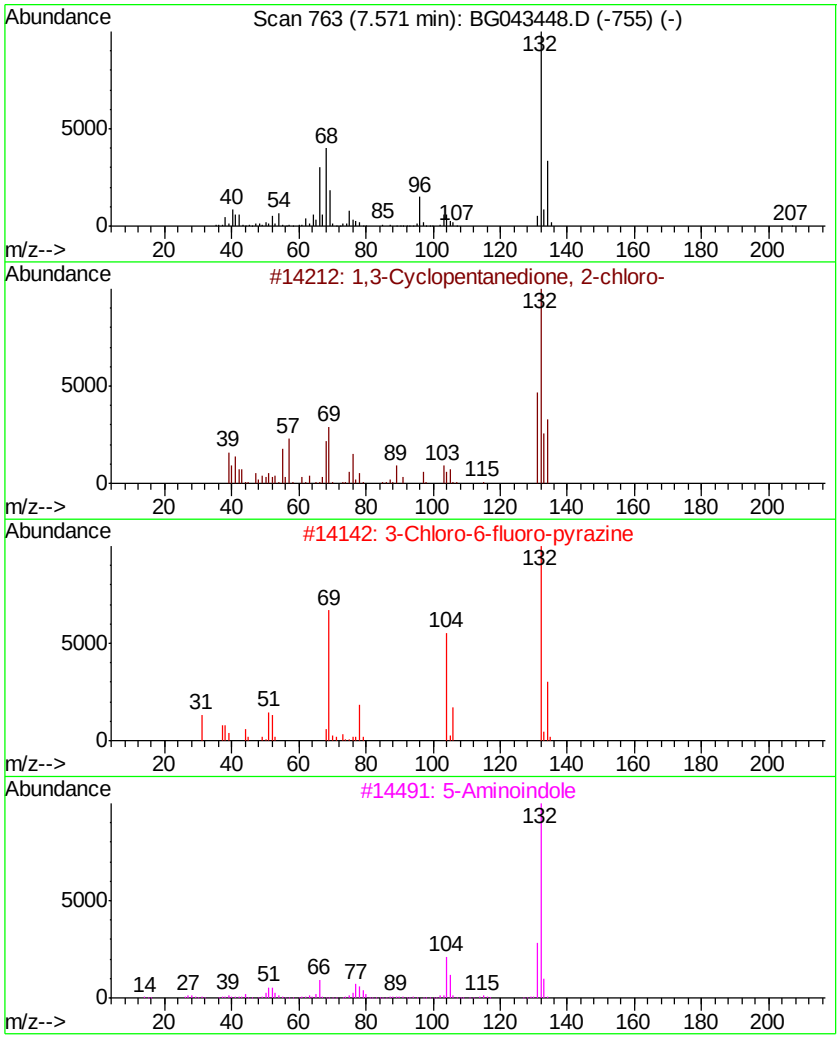
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

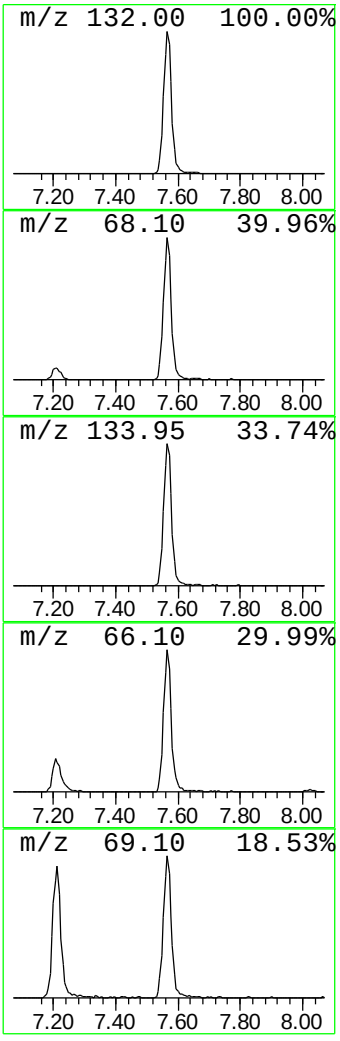
****

Peak Number 3 unknown7.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	73.57 ng	1012140	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	32
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	22
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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Acq On : 1 Nov 2019 00:13
Operator : JU
Sample : K5620-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-25-S

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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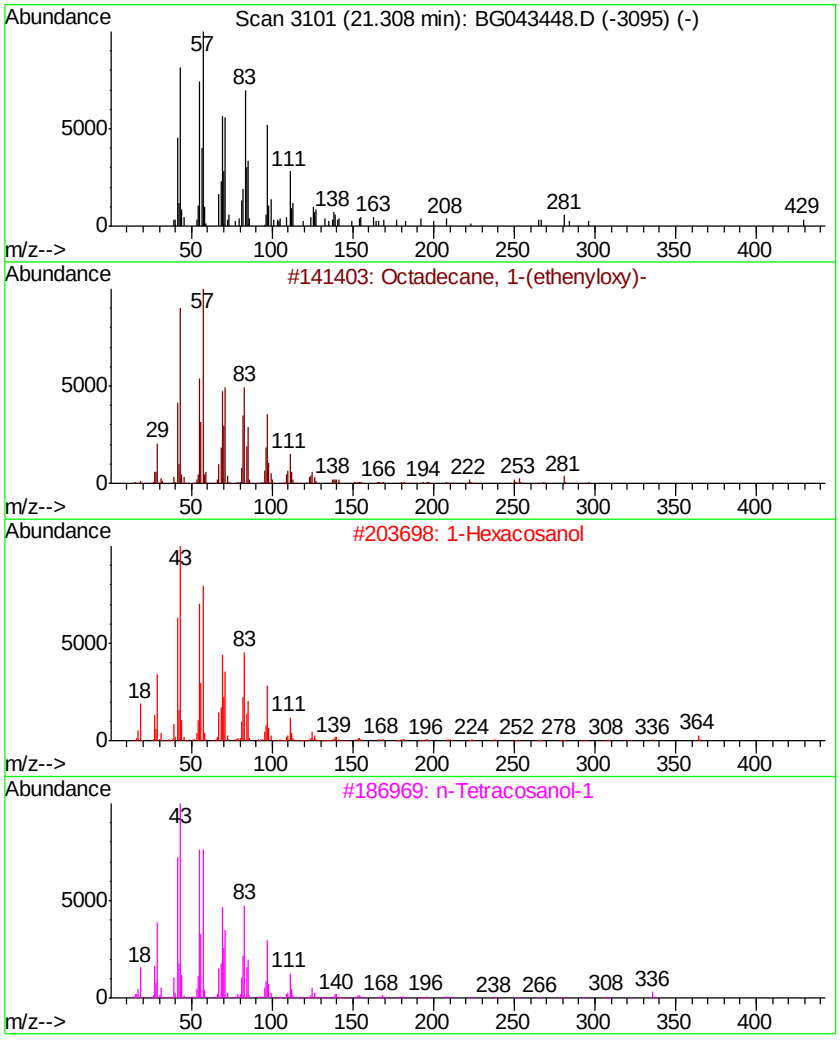
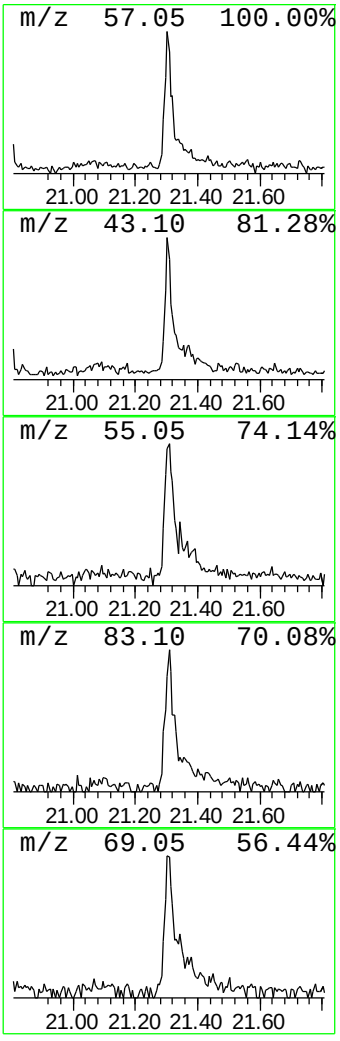
Peak Number 5 Octadecane, 1-(ethenyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	3.29 ng	131385	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	91
2	1-Hexacosanol	382	C26H54O	000506-52-5	87
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
4	Cyclooctacosane	392	C28H56	000297-24-5	87
5	1-Tricosene	322	C23H46	018835-32-0	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
Data File : BG043448.D
Acq On : 1 Nov 2019 00:13
Operator : JU
Sample : K5620-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-25-S

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

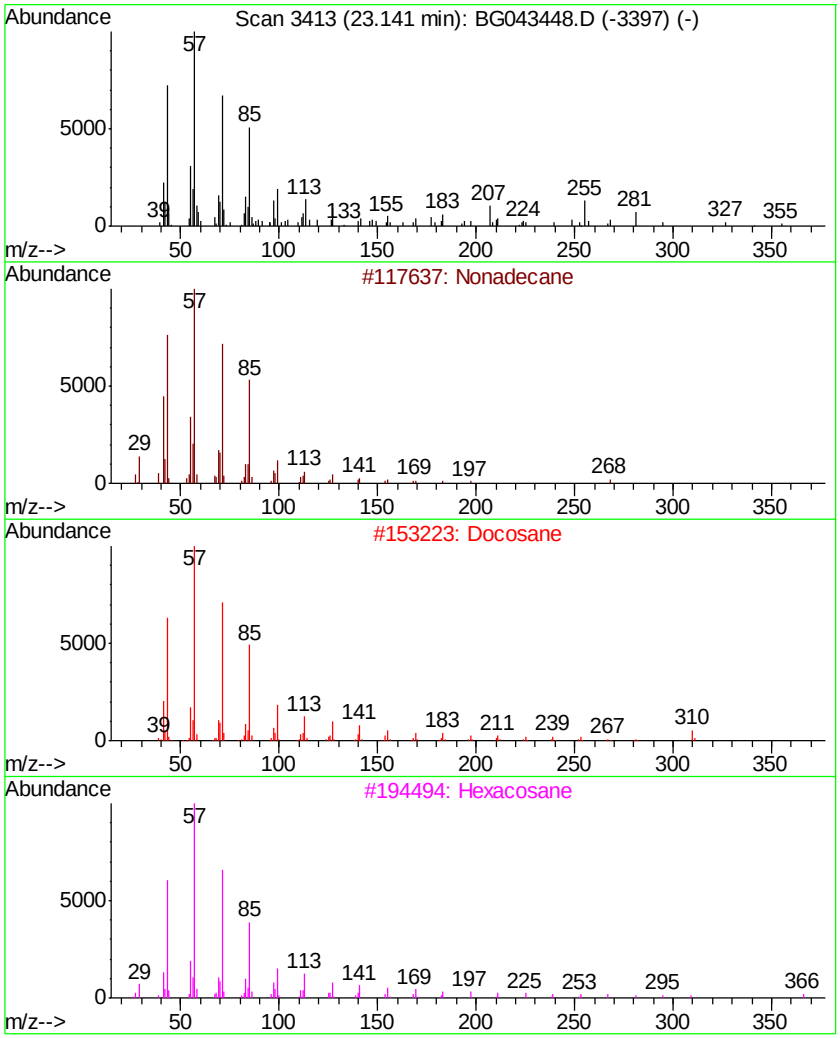
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

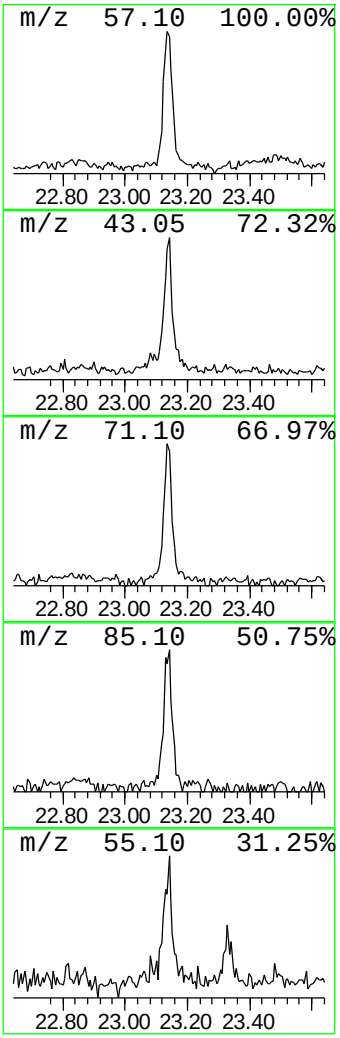
****

Peak Number 6 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.14	4.39 ng	175043	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Docosane	310	C22H46	000629-97-0	74
3	Hexacosane	366	C26H54	000630-01-3	72
4	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	72
5	5-Butyl-5-ethylheptadecane	324	C23H48	1000360-43-0	72





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Sample : K5620-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-25-S

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

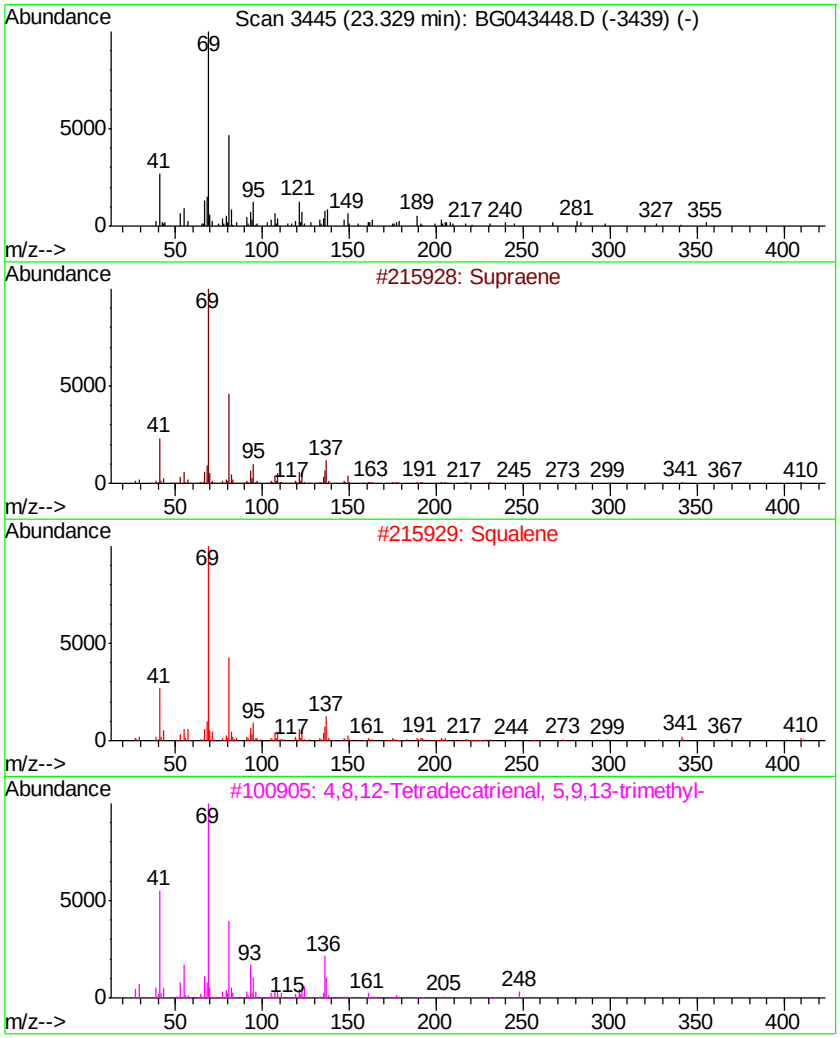
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

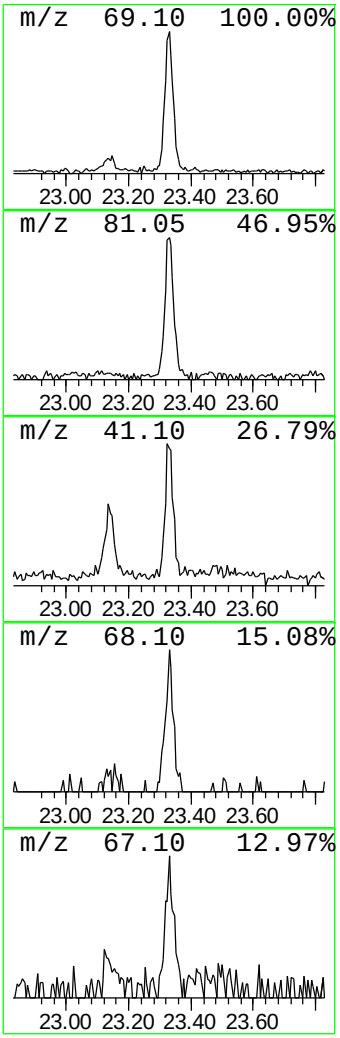
****

Peak Number 7 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.33	2.49 ng	114323	Perylene-d12	24.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	80
2	Squalene	410	C30H50	000111-02-4	72
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
4	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	59
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	003790-71-4	59





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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-25-S

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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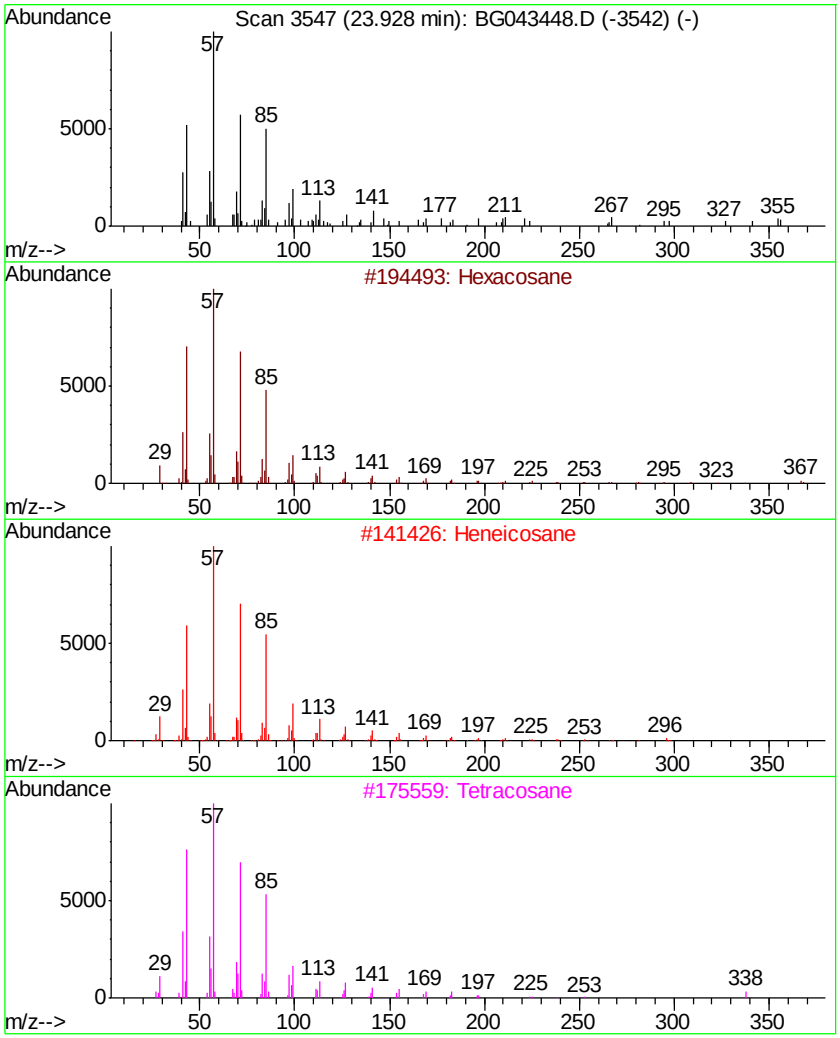
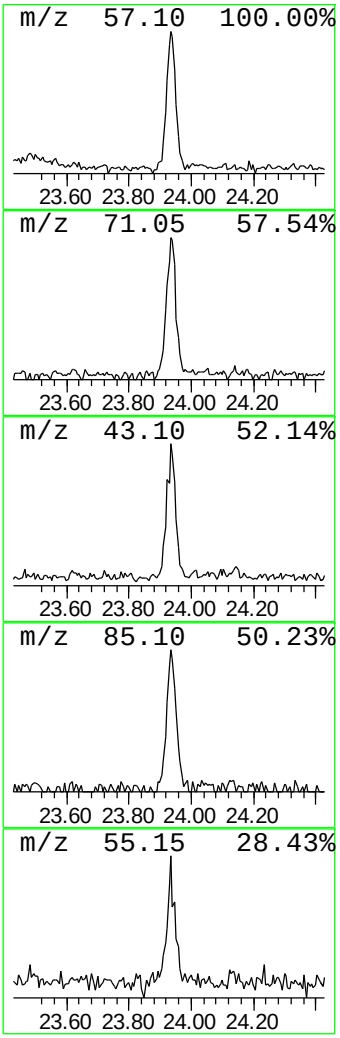
Peak Number 8 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.93	2.04 ng	93598	Perylene-d12	24.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Tetracosane	338	C24H50	000646-31-1	90
4	2-methyloctacosane	408	C29H60	1000376-72-8	87
5	Octacosane	394	C28H58	000630-02-4	87





Tentatively Identified Compound (LSC) summary

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ClientSampleId : TP-25-S

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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
Butane, 2-methoxy...	3.20	13.3	ng	182797	1	8.02	275159	20.0
2-Pentanone, 4-hy...	5.13	15.0	ng	206614	1	8.02	275159	20.0
unknown7.57	7.57	73.6	ng	1012140	1	8.02	275159	20.0
Octadecane, 1-(et...	21.31	3.3	ng	131385	5	21.66	797935	20.0
Nonadecane	23.14	4.4	ng	175043	5	21.66	797935	20.0
Supraene	23.33	2.5	ng	114323	6	24.86	918835	20.0
Hexacosane	23.93	2.0	ng	93598	6	24.86	918835	20.0