LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG032019\
Data File : BG040051.D
Acq On : 21 Mar 2019 1:06
Operator : JU/SJ
Sample : K1972-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-10-031519

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-BG030419.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	3.197	13	18	26	rBV	172692	305390	9.66%	1.714%
2	3.268	26	30	47	rVB	450578	642738	20.32%	3.607%
3	5.688	434	442	451	rBV	424074	673147	21.28%	3.778%
4	7.286	707	714	724	rVB	286148	491524	15.54%	2.758%
5	7.668	772	779	787	rBV	741771	1279422	40.45%	7.180%
6	8.144	853	860	870	rVB	160391	270784	8.56%	1.520%
7	8.467	907	915	924	rVB	623921	1082429	34.22%	6.074%
8	9.318	1051	1060	1069	rBV	571751	1032859	32.66%	5.796%
9	10.963	1332	1340	1346	rBV	225367	398963	12.61%	2.239%
10	13.389	1746	1753	1760	rBV	1537977	2402879	75.97%	13.484%
11	14.770	1982	1988	1997	rVB2	347474	568963	17.99%	3.193%
12	16.256	2234	2241	2254	rBV	1211253	1852016	58.56%	10.393%
13	17.513	2448	2455	2461	rBV2	451188	697521	22.05%	3.914%
14	18.365	2595	2600	2607	rBV4	66246	119393	3.77%	0.670%
15	19.628	2811	2815	2820	rBV2	47068	71101	2.25%	0.399%
16	20.104	2890	2896	2902	rBV	2348126	3162830	100.00%	17.749%
17	21.796	3178	3184	3194	rVB2	456574	759229	24.00%	4.261%
18	21.937	3204	3208	3213	rVB2	50554	72850	2.30%	0.409%
19	22.559	3309	3314	3322	rVB	84264	142750	4.51%	0.801%
20	23.276	3429	3436	3443	rVB	117352	239363	7.57%	1.343%
21	24.104	3569	3577	3587	rVB	112561	253567	8.02%	1.423%
22	25.085	3736	3744	3748	rBV3	85994	227228	7.18%	1.275%
23	25.156	3748	3756	3768	rVB3	246656	760141	24.03%	4.266%
24	26.254	3934	3943	3954	rVB2	66230	197485	6.24%	1.108%
25	27.658	4173	4182	4194	rBV5	30968	115168	3.64%	0.646%

Sum of corrected areas: 17819740

LSC Report - Integrated Chromatogram

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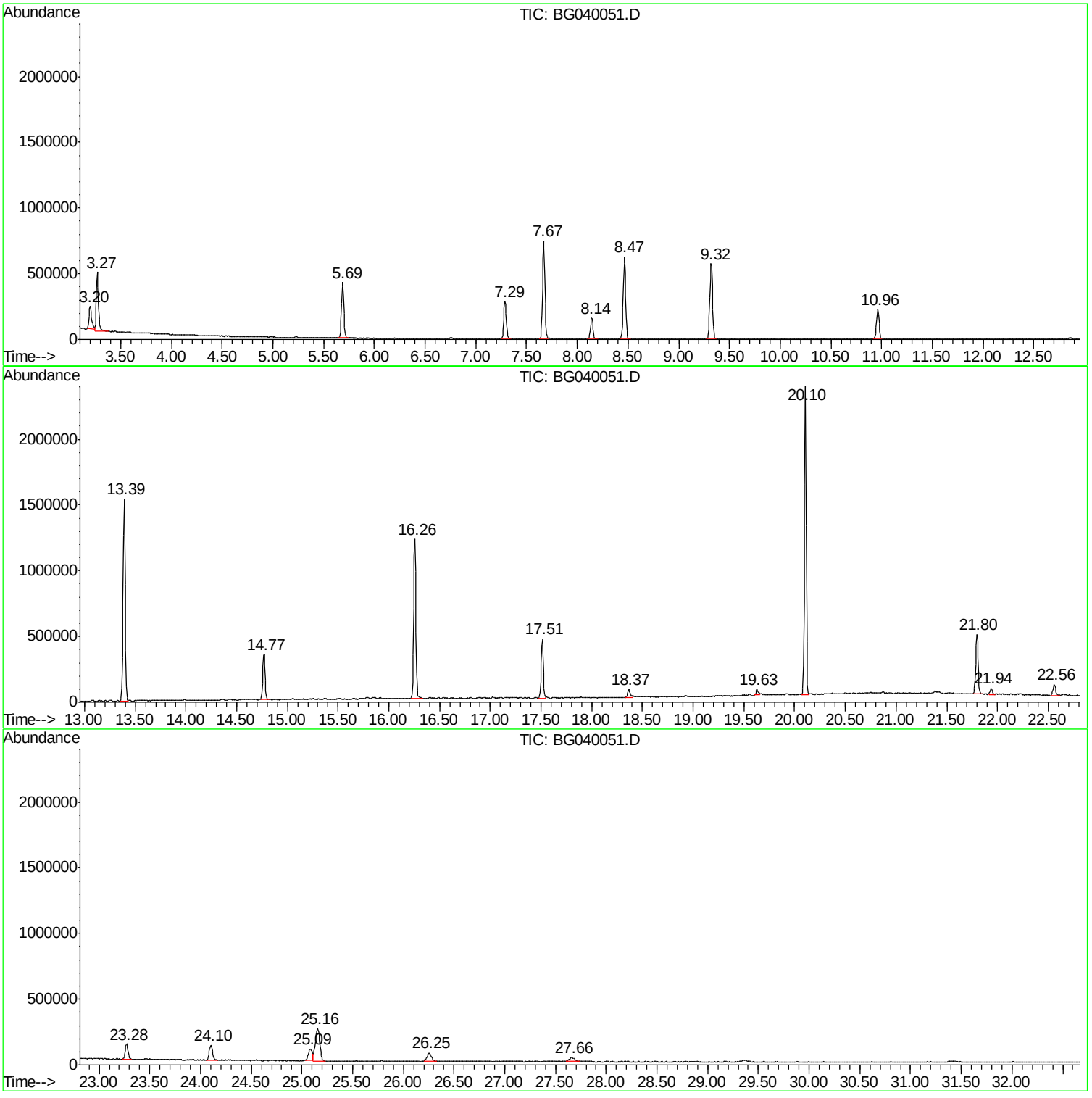
Operator : JU/SJ
Sample : K1972-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TW-10-031519

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.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 : BG040051.D
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ClientSampleId : TW-10-031519

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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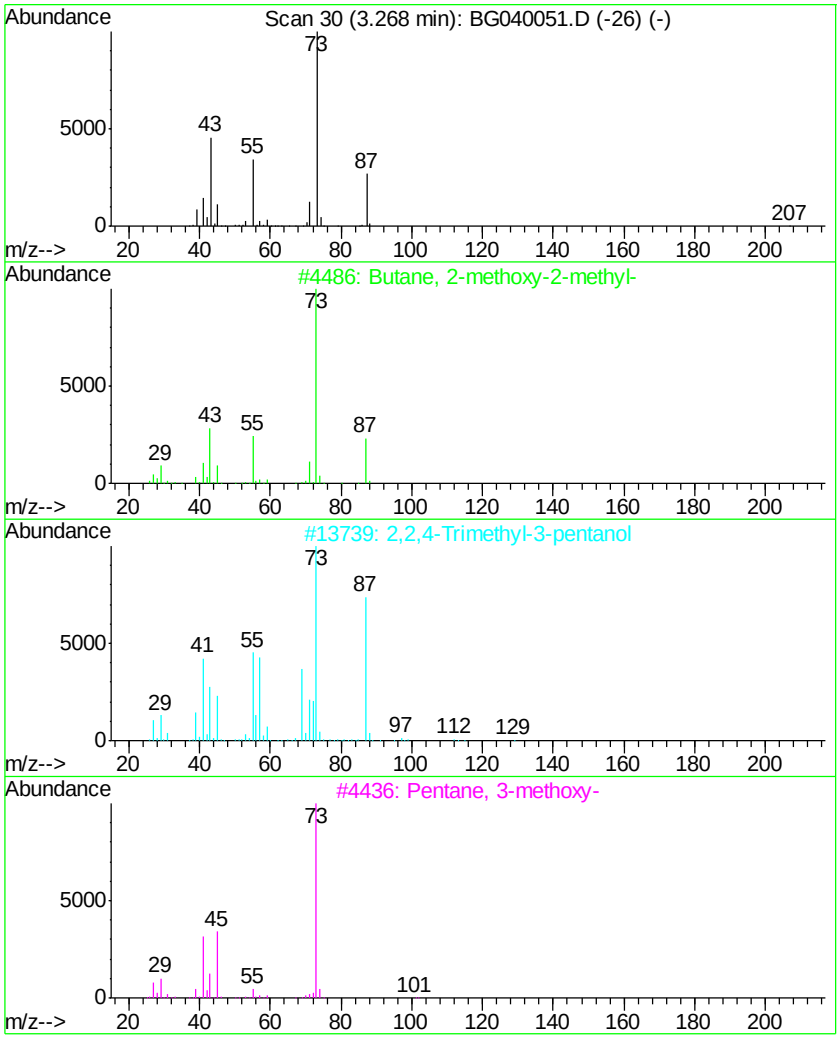
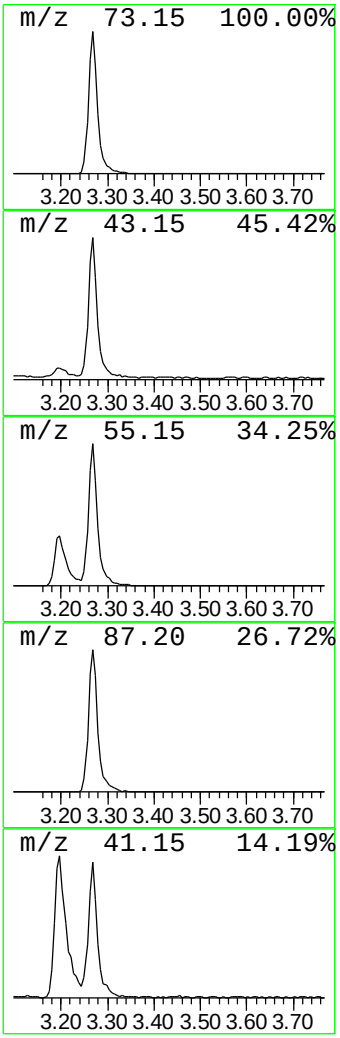
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.27	47.47 ng	642738	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

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Operator : JU/SJ
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-10-031519

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.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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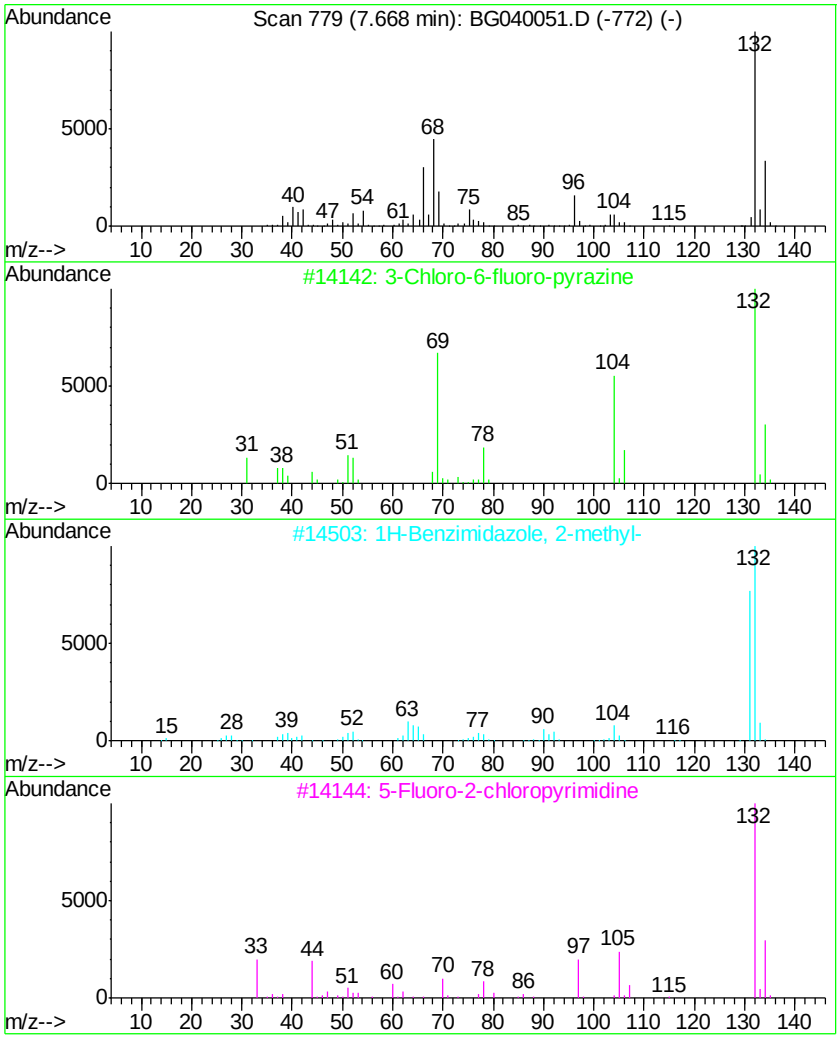
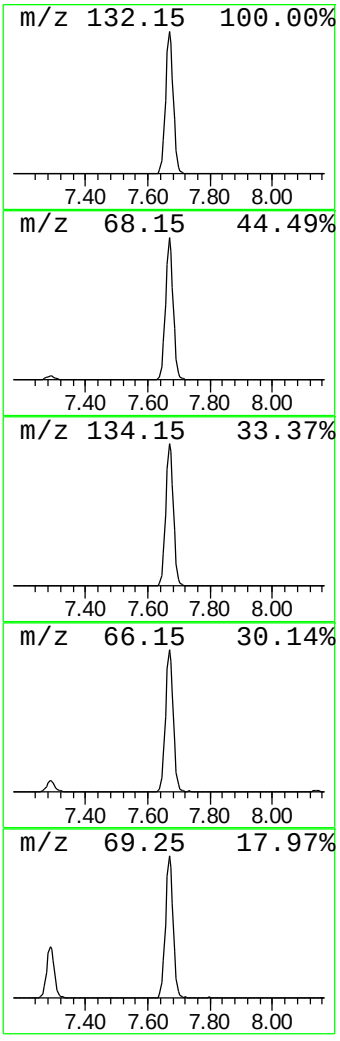
Peak Number 3 unknown7.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.67	94.50 ng	1279420	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG032019\
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Operator : JU/SJ
Sample : K1972-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-10-031519

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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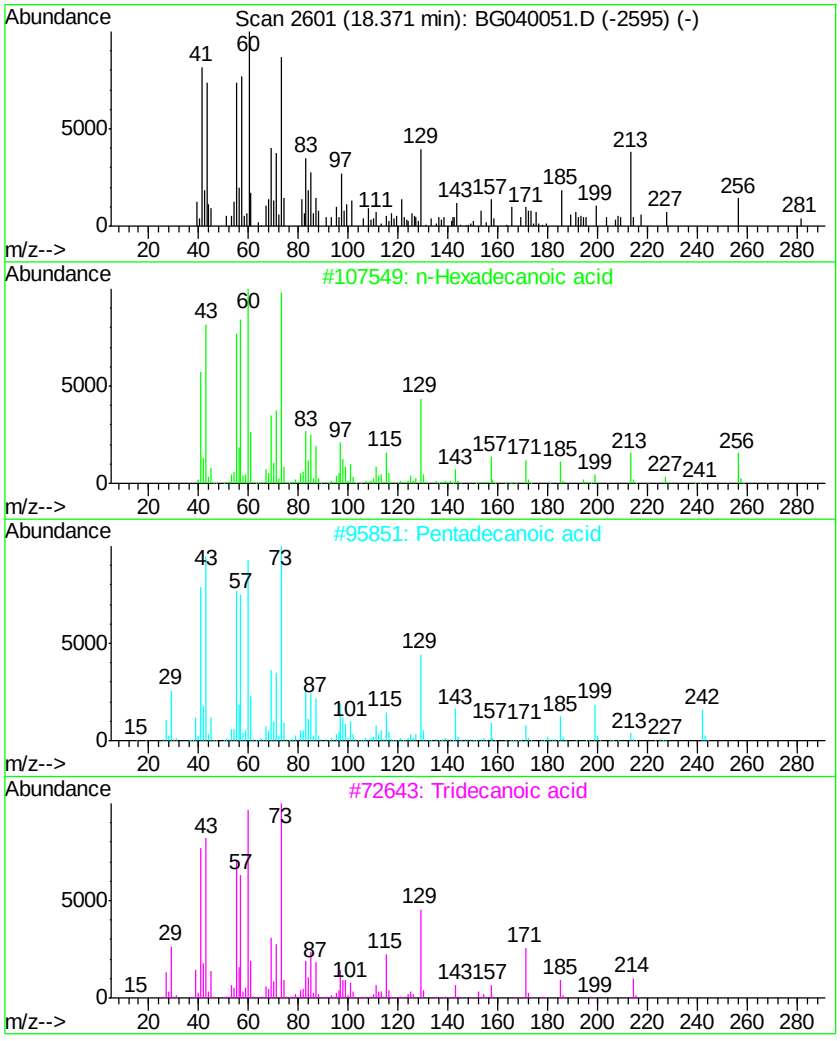
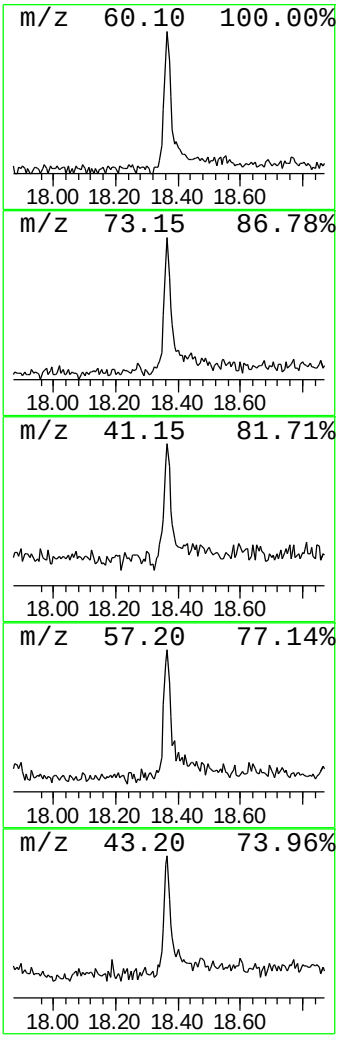
Peak Number 5 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.37	3.42 ng	119393	Phenanthrene-d10	17.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Library Search Compound Report

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Data File : BG040051.D
Acq On : 21 Mar 2019 1:06
Operator : JU/SJ
Sample : K1972-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-10-031519

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.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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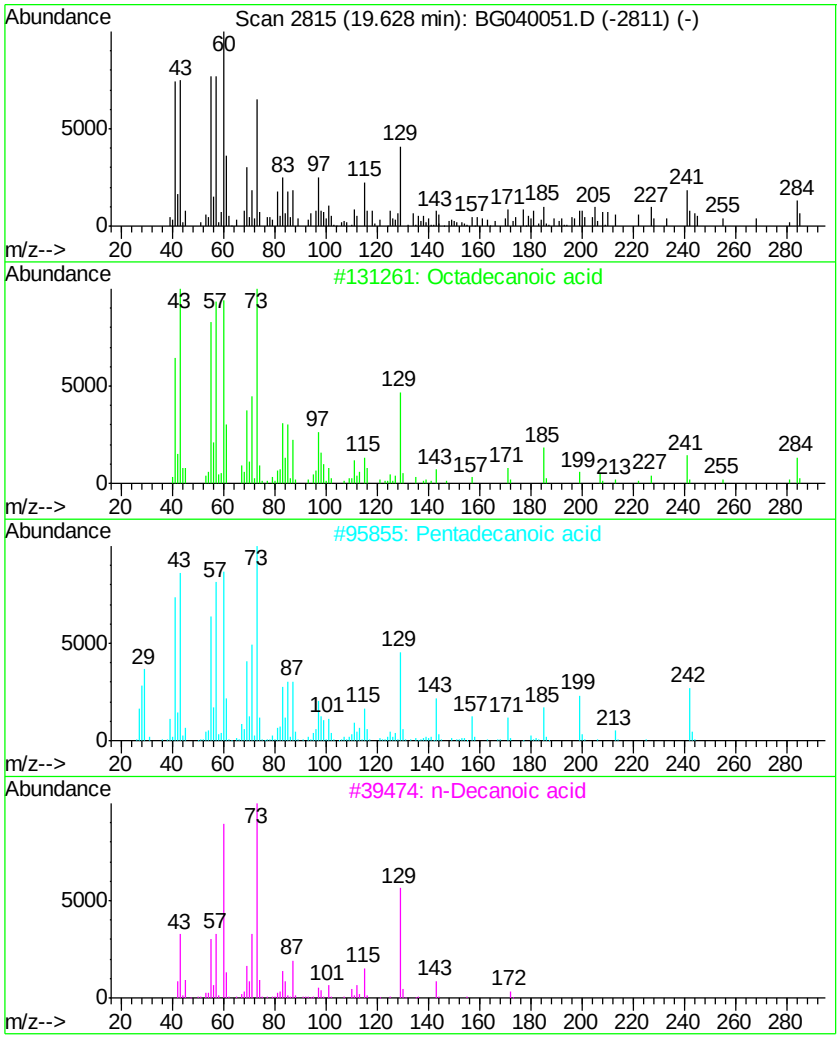
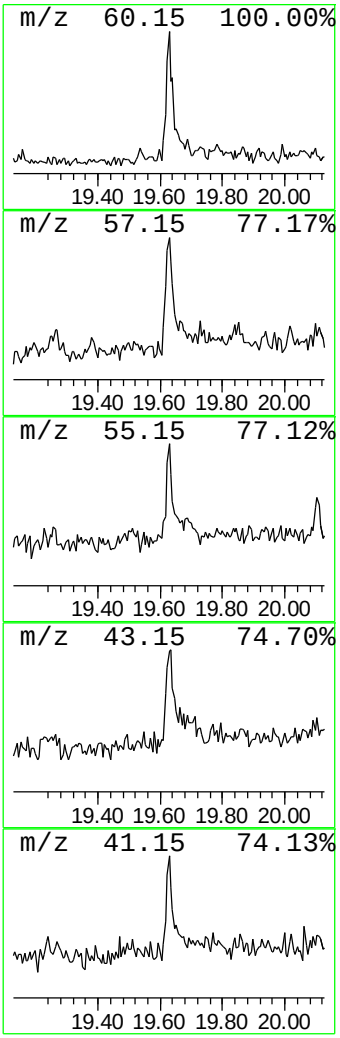
Peak Number 6 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.63	2.04 ng	71101	Phenanthrene-d10	17.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	62
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	51
3	n-Decanoic acid	172	C10H20O2	000334-48-5	50
4	.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	38
5	Dodecanoic acid	200	C12H24O2	000143-07-7	38





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Sample : K1972-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-10-031519

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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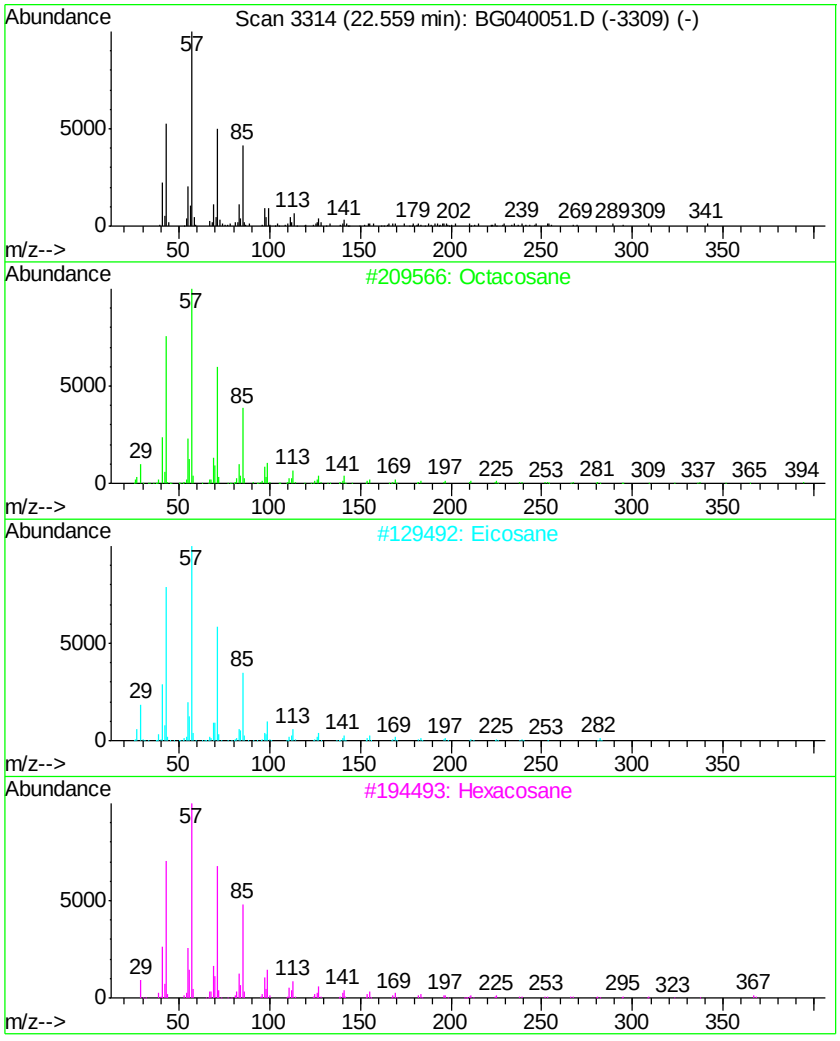
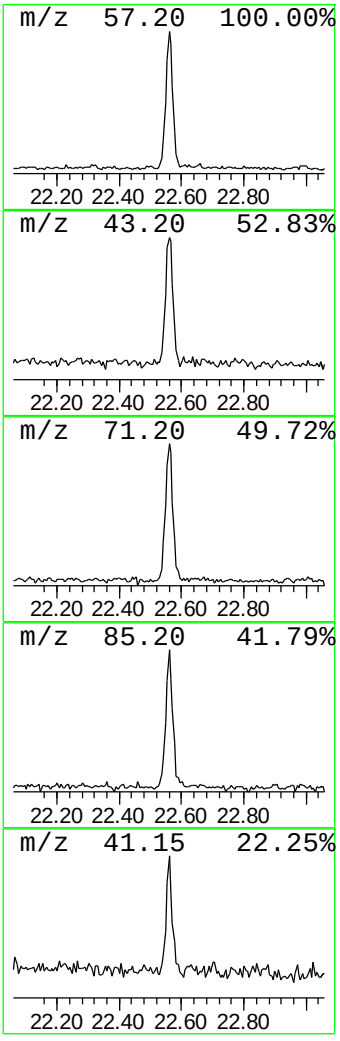
Peak Number 7 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.56	3.76 ng	142750	Chrysene-d12	21.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	80
2	Eicosane	282	C20H42	000112-95-8	80
3	Hexacosane	366	C26H54	000630-01-3	74
4	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	72
5	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	60





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Sample : K1972-03
Misc :
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Instrument : BNA_G
ClientSampleId : TW-10-031519

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

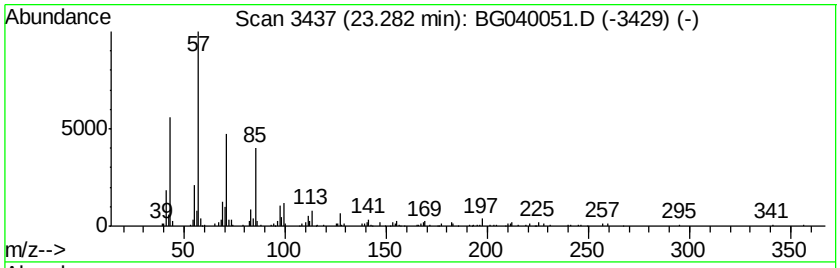
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

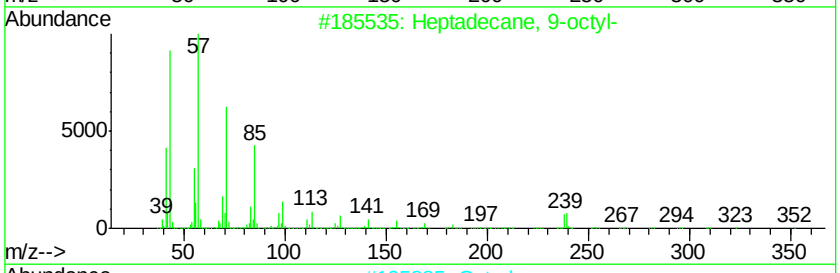
****

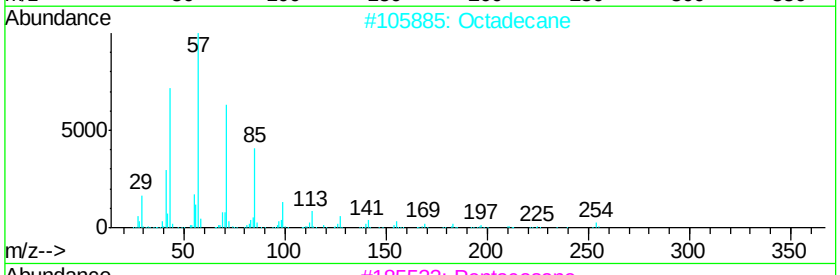
Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 6

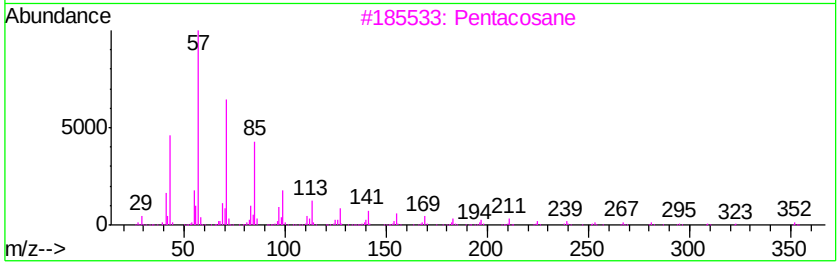
R.T.	EstConc	Area	Relative to ISTD	R.T.
23.28	6.31 ng	239363	Chrysene-d12	21.80

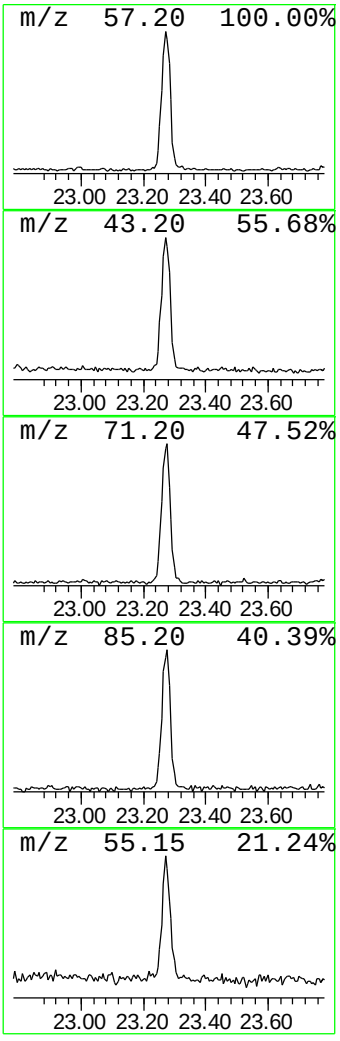
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Octadecane	254	C18H38	000593-45-3	91
3	Pentacosane	352	C25H52	000629-99-2	91
4	Tetracosane	338	C24H50	000646-31-1	90
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90











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Instrument : BNA_G
ClientSampleId : TW-10-031519

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

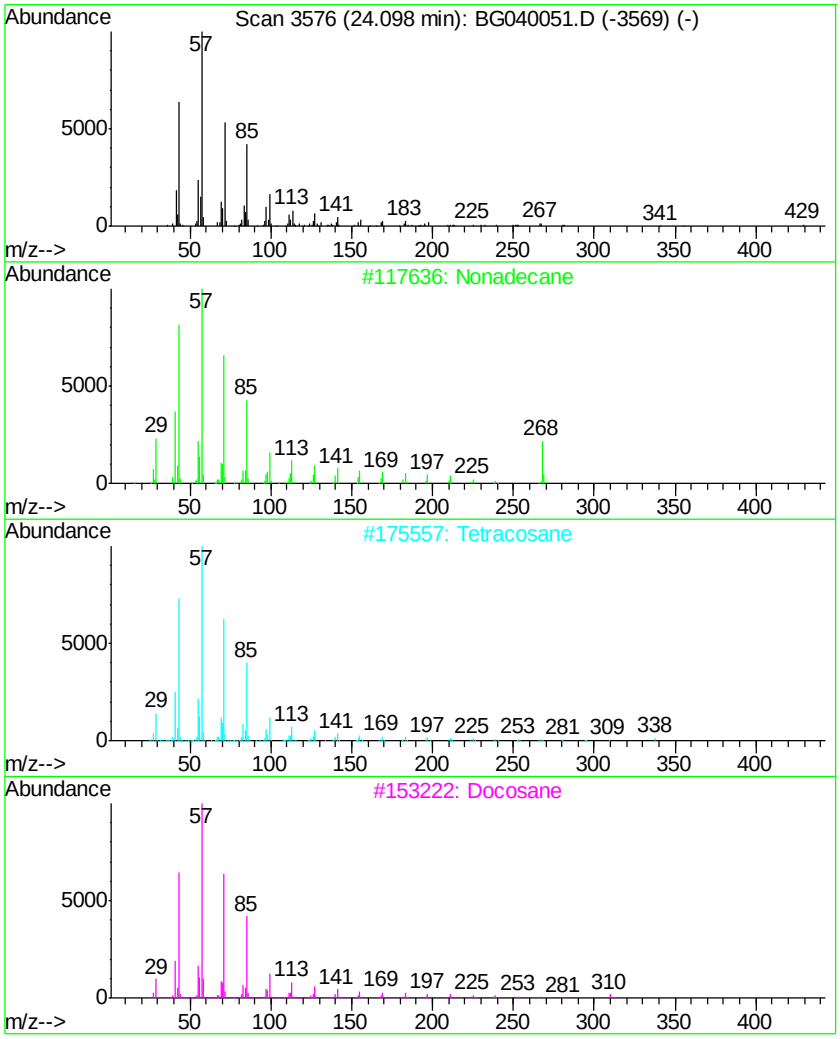
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

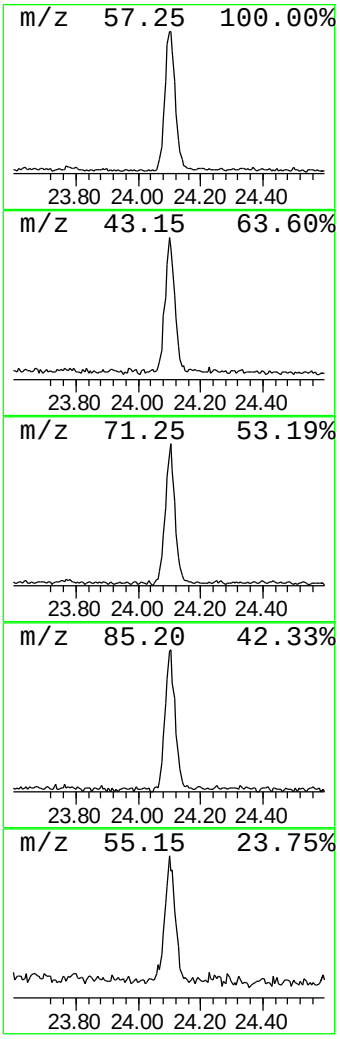
****

Peak Number 9 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.10	6.67 ng	253567	Perylene-d12	25.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Tetracosane	338	C24H50	000646-31-1	91
3	Docosane	310	C22H46	000629-97-0	91
4	Octadecane	254	C18H38	000593-45-3	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





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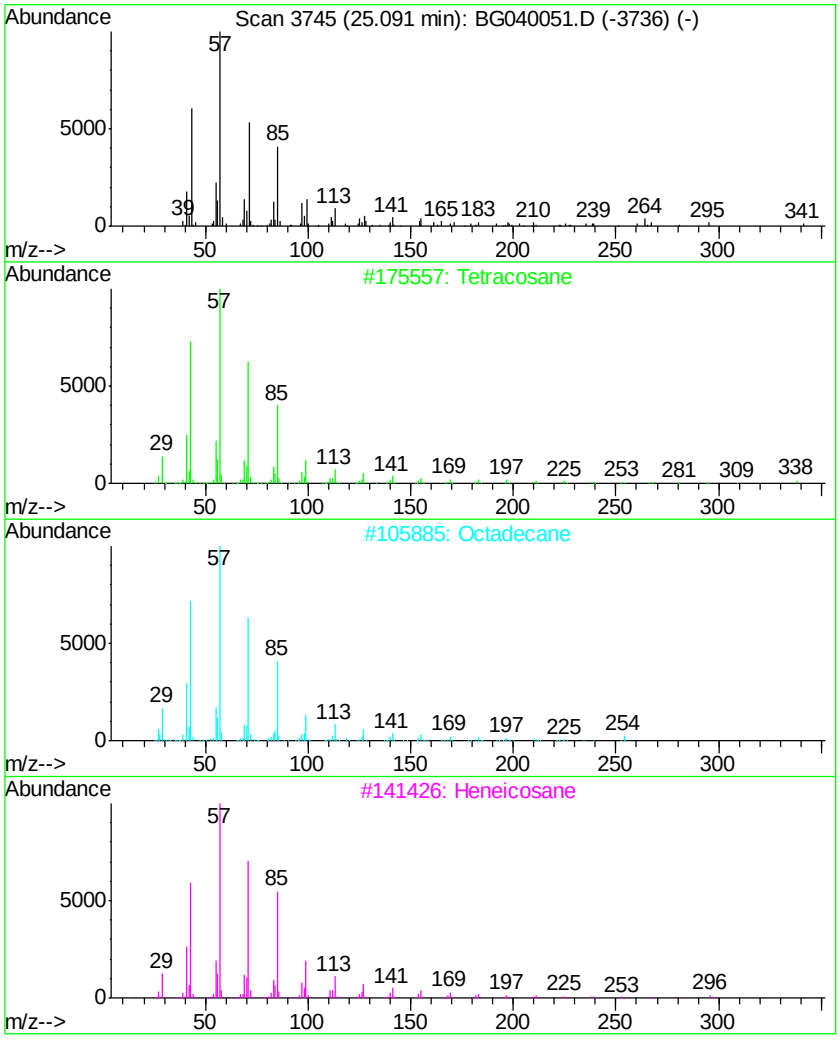
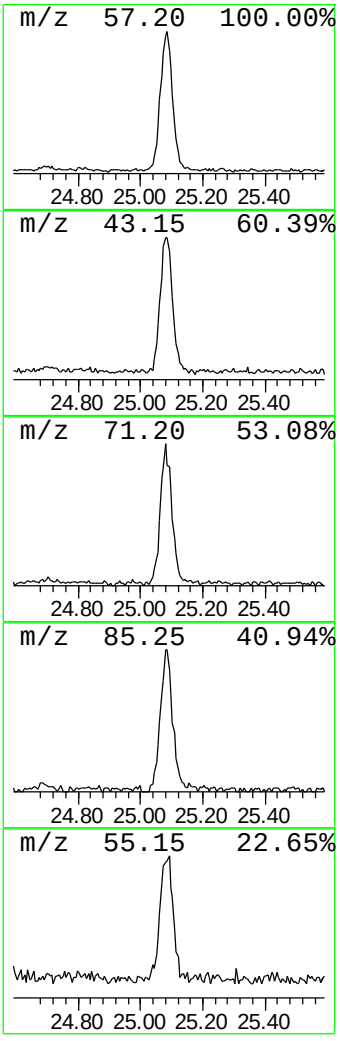
Peak Number 10 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.09	5.98 ng	227228	Perylene-d12	25.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	Octadecane	254	C18H38	000593-45-3	87
3	Heneicosane	296	C21H44	000629-94-7	81
4	Octacosane	394	C28H58	000630-02-4	76
5	Nonadecane	268	C19H40	000629-92-5	74





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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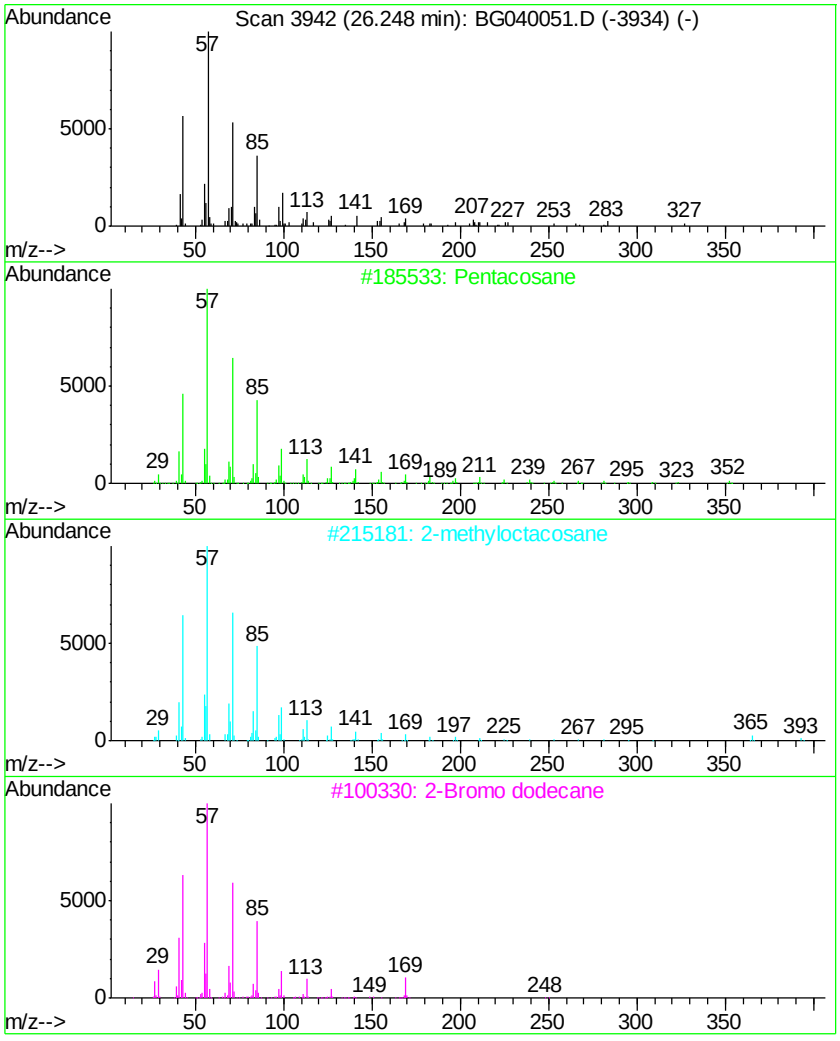
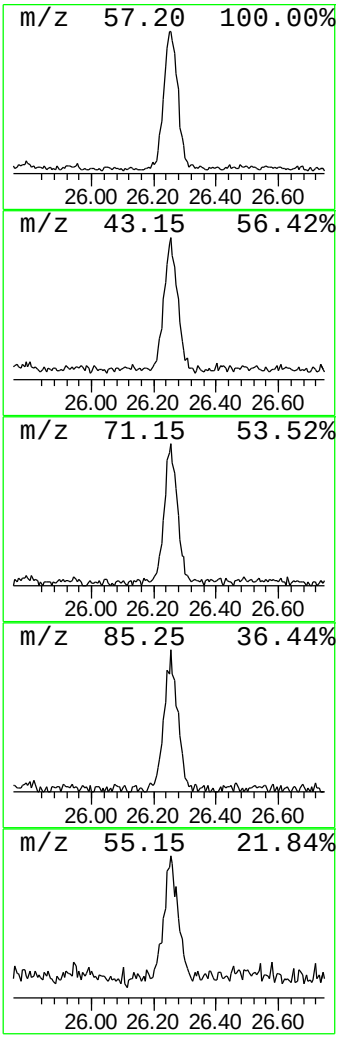
Peak Number 11 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.25	5.20 ng	197485	Perylene-d12	25.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	87
2	2-methyloctacosane	408	C29H60	1000376-72-8	87
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	80
4	Docosane	310	C22H46	000629-97-0	80
5	Triacontane	422	C30H62	000638-68-6	72





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Data File : BG040051.D
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Operator : JU/SJ
Sample : K1972-03
Misc :
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Instrument : BNA_G
ClientSampleId : TW-10-031519

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

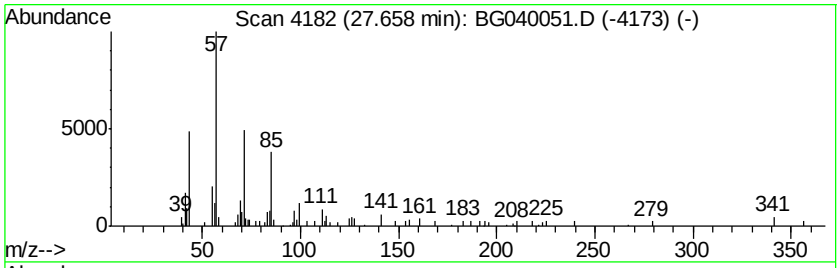
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

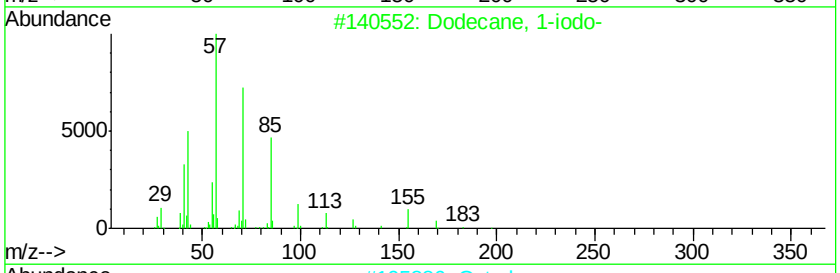
****

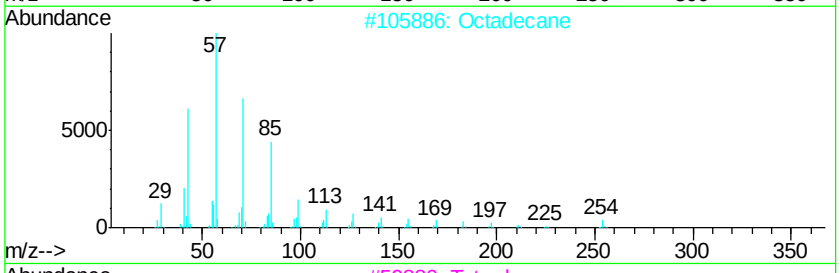
Peak Number 12 Dodecane, 1-iodo- Concentration Rank 11

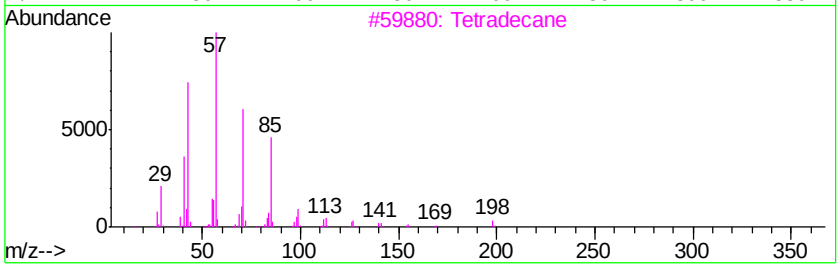
R.T.	EstConc	Area	Relative to ISTD	R.T.
27.66	3.03 ng	115168	Perylene-d12	25.16

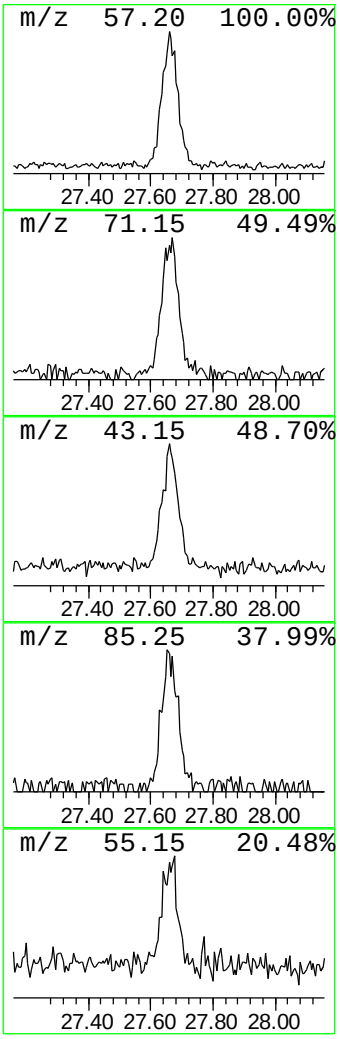
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72
2	Octadecane	254	C18H38	000593-45-3	64
3	Tetradecane	198	C14H30	000629-59-4	64
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	64
5	Tetracosane	338	C24H50	000646-31-1	64











Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG032019\
Data File : BG040051.D
Acq On : 21 Mar 2019 1:06
Operator : JU/SJ
Sample : K1972-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-10-031519

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.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...	3.27	47.5	ng	642738	1	8.14	270784	20.0
unknown7.67	7.67	94.5	ng	1279420	1	8.14	270784	20.0
n-Hexadecanoic acid	18.37	3.4	ng	119393	4	17.51	697521	20.0
Octadecanoic acid	19.63	2.0	ng	71101	4	17.51	697521	20.0
Octacosane	22.56	3.8	ng	142750	5	21.80	759229	20.0
Heptadecane, 9-oc...	23.28	6.3	ng	239363	5	21.80	759229	20.0
Nonadecane	24.10	6.7	ng	253567	6	25.16	760141	20.0
Tetracosane	25.09	6.0	ng	227228	6	25.16	760141	20.0
Pentacosane	26.25	5.2	ng	197485	6	25.16	760141	20.0
Dodecane, 1-iodo-	27.66	3.0	ng	115168	6	25.16	760141	20.0