LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100219\
Data File : BG042990.D
Acq On : 2 Oct 2019 18:27
Operator : JU
Sample : K5154-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-106S

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-BG092519.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	3.183	8	16	25	rBV2	242000	707637	12.04%	2.377%
2	3.265	25	30	45	rVB	379627	752456	12.81%	2.528%
3	5.656	430	437	450	rBV	893849	1494996	25.44%	5.022%
4	7.237	696	706	717	rBV	647866	1201754	20.45%	4.037%
5	7.607	761	769	781	rBV	1268398	2241729	38.15%	7.530%
6	8.071	840	848	855	rBV	265184	451069	7.68%	1.515%
7	8.394	893	903	912	rBV	961121	1684210	28.66%	5.658%
8	9.229	1037	1045	1057	rBV	783407	1441621	24.53%	4.843%
9	10.874	1317	1325	1334	rBV	312215	583132	9.92%	1.959%
10	11.778	1471	1479	1490	rBV3	38107	93899	1.60%	0.315%
11	13.312	1733	1740	1756	rBV	2185144	3520221	59.91%	11.825%
12	14.135	1874	1880	1886	rBV	128590	191305	3.26%	0.643%
13	14.687	1964	1974	1984	rBV	547102	882179	15.01%	2.963%
14	15.092	2038	2043	2053	rBV	45455	73272	1.25%	0.246%
15	16.173	2218	2227	2242	rBV	2092782	3224801	54.88%	10.833%
16	17.431	2434	2441	2450	rBV2	657553	1054948	17.95%	3.544%
17	18.318	2587	2592	2598	rBV	204554	287888	4.90%	0.967%
18	19.587	2803	2808	2813	rBV2	115900	156328	2.66%	0.525%
19	20.039	2879	2885	2897	rBV	4320530	5875815	100.00%	19.738%
20	21.350	3104	3108	3111	rBV	51287	79429	1.35%	0.267%
21	21.702	3161	3168	3177	rBV2	715776	1239740	21.10%	4.164%
22	21.896	3197	3201	3207	rVB	69498	106990	1.82%	0.359%
23	22.507	3301	3305	3311	rVB2	90415	138093	2.35%	0.464%
24	23.206	3415	3424	3431	rBV2	121372	253597	4.32%	0.852%
25	24.011	3555	3561	3572	rVB	127444	276739	4.71%	0.930%
26	24.922	3707	3716	3733	rVB2	454868	1553101	26.43%	5.217%
27	26.103	3910	3917	3927	rVB5	69384	202515	3.45%	0.680%

Sum of corrected areas: 29769464

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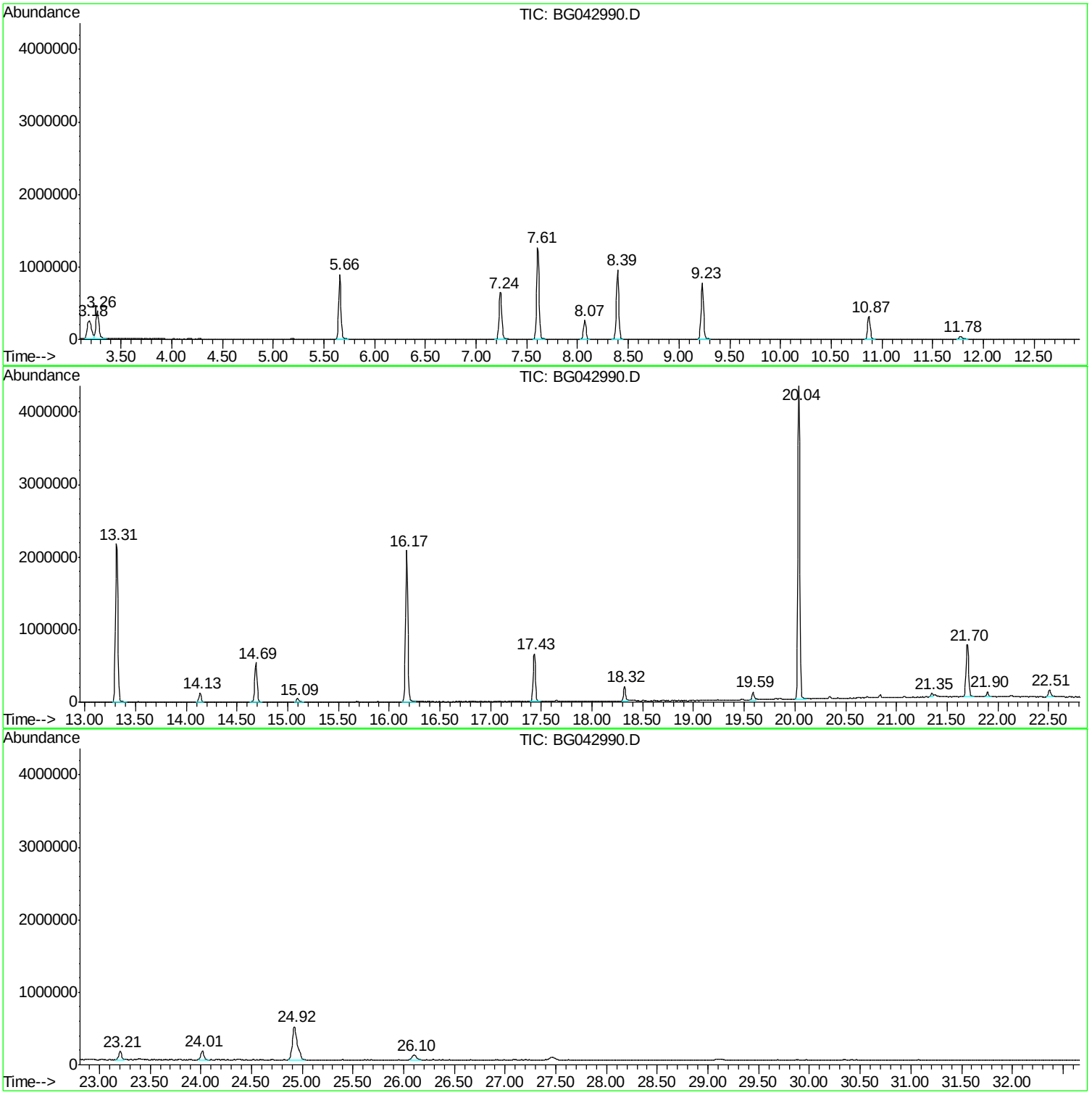
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-106S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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

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Data File : BG042990.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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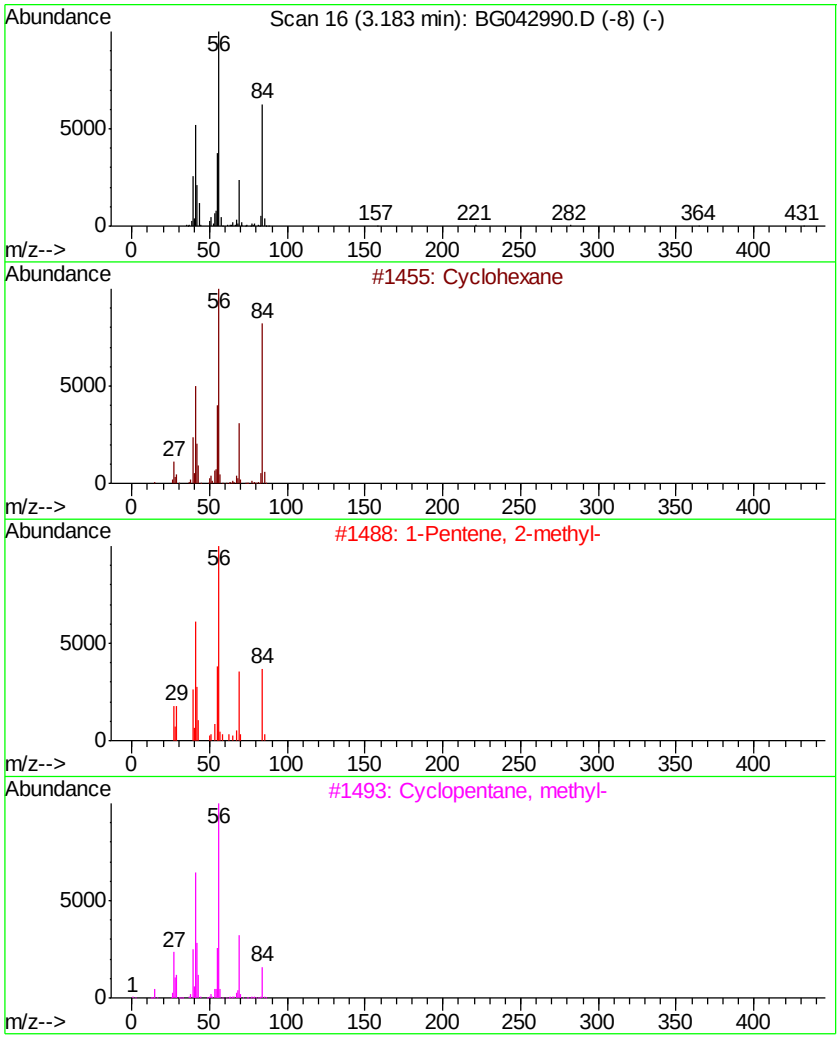
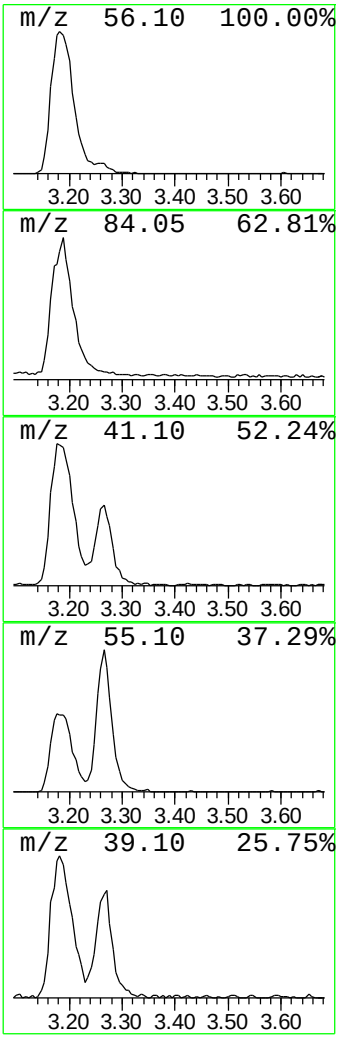
****

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	31.38 ng	707637	1,4-Dichlorobenzene-d4	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	94
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	53
4	1-Hexene	84	C6H12	000592-41-6	50
5	Cyanic acid, 2-methylpropyl ester	99	C5H9NO	001768-25-8	45





Library Search Compound Report

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Data File : BG042990.D
Acq On : 2 Oct 2019 18:27
Operator : JU
Sample : K5154-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-106S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

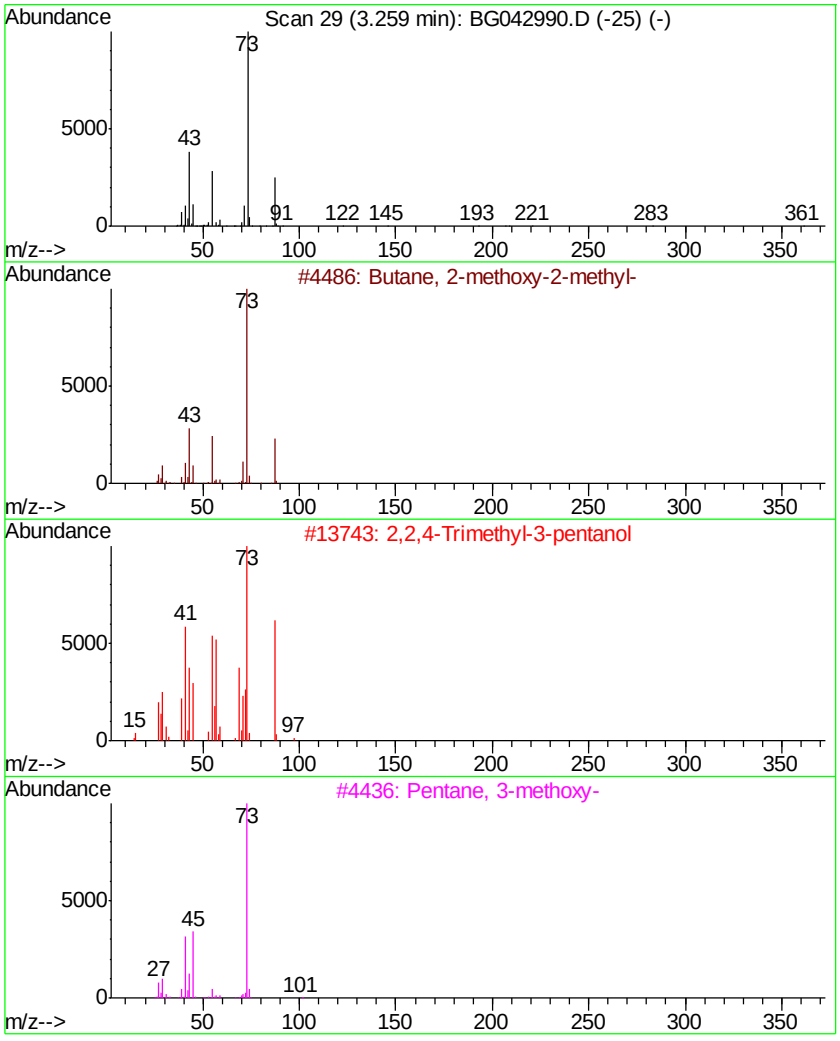
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

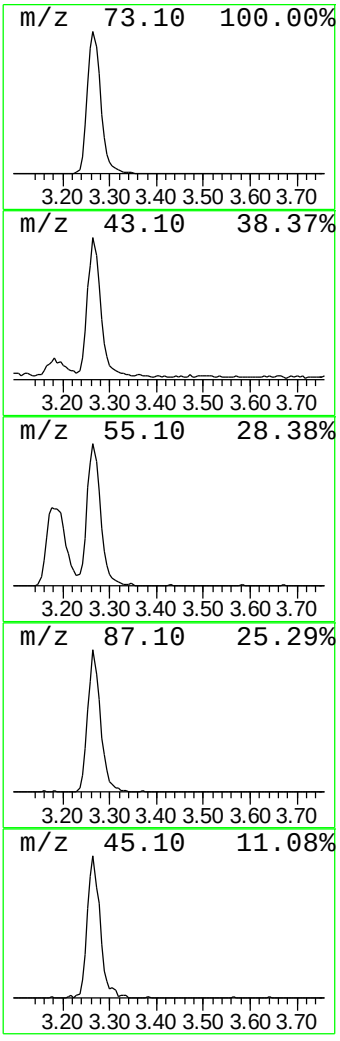
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.26	33.36 ng	752456	1,4-Dichlorobenzene-d4	8.07

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	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100219\
Data File : BG042990.D
Acq On : 2 Oct 2019 18:27
Operator : JU
Sample : K5154-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-106S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

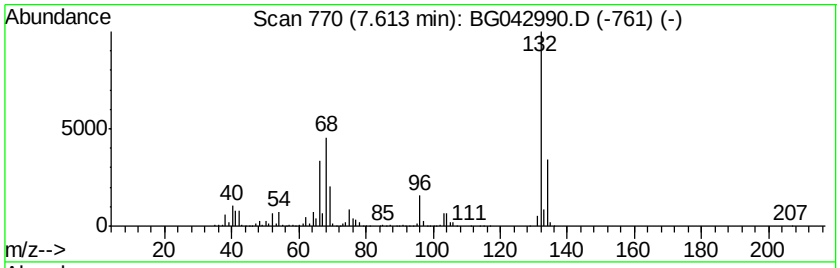
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

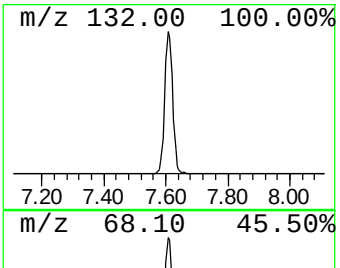
****

Peak Number 3 unknown7.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.61	99.40 ng	2241730	1,4-Dichlorobenzene-d4	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





Library Search Compound Report

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Data File : BG042990.D
Acq On : 2 Oct 2019 18:27
Operator : JU
Sample : K5154-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-106S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

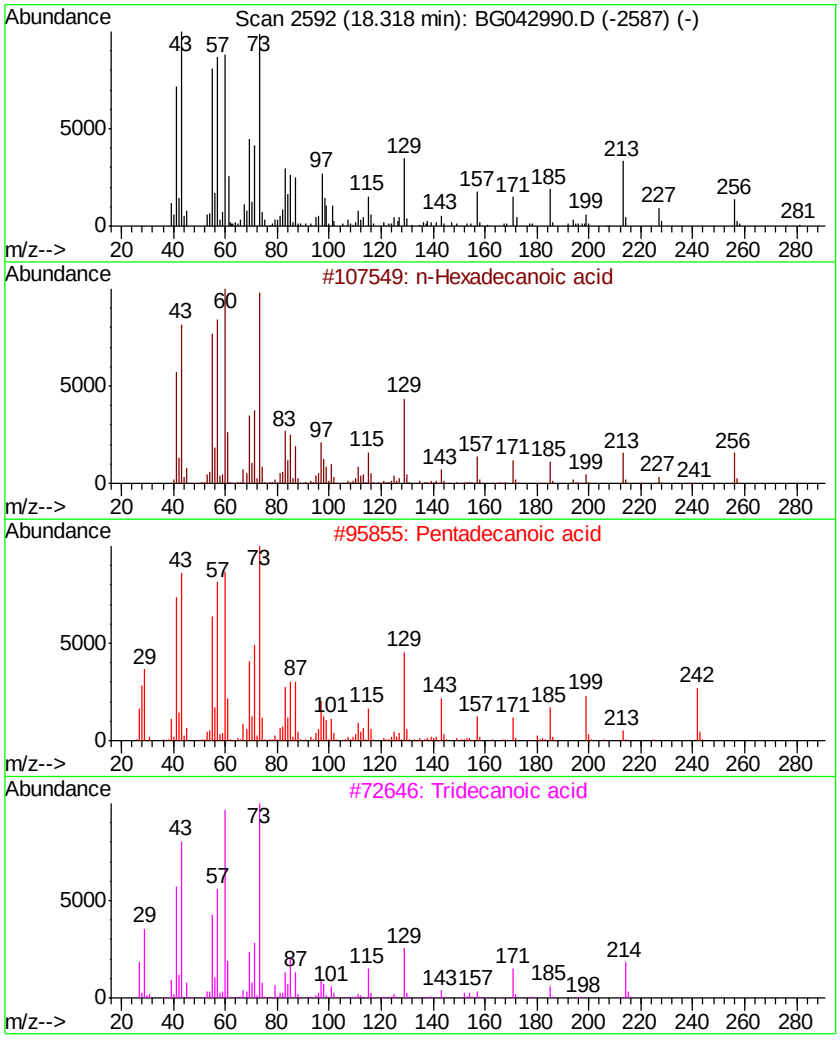
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

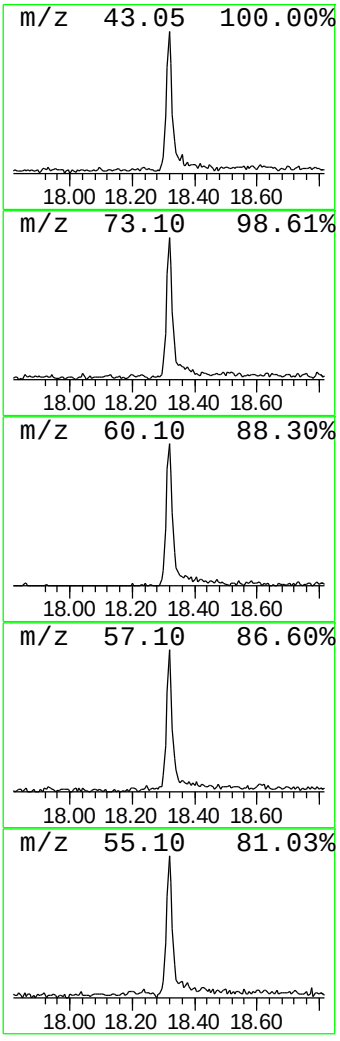
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.32	5.46 ng	287888	Phenanthrene-d10	17.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3	Tridecanoic acid	214	C13H26O2	000638-53-9	70
4	n-Decanoic acid	172	C10H20O2	000334-48-5	52
5	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	18





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100219\
Data File : BG042990.D
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Operator : JU
Sample : K5154-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-106S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

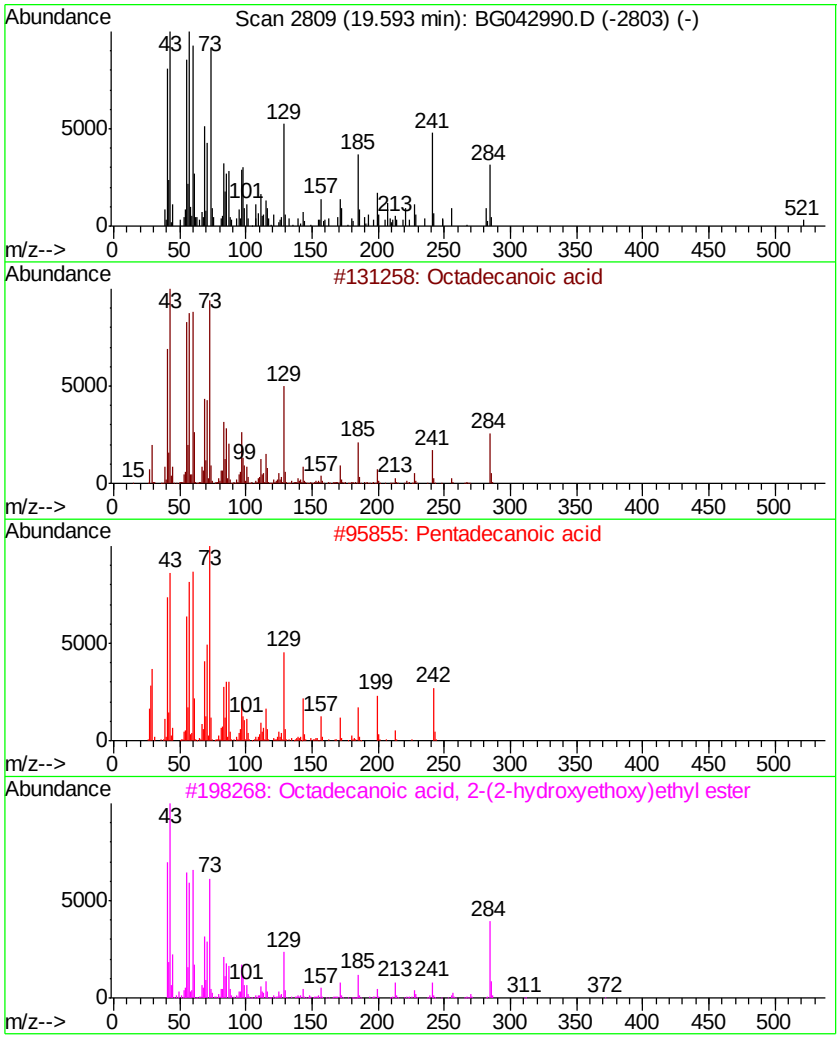
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

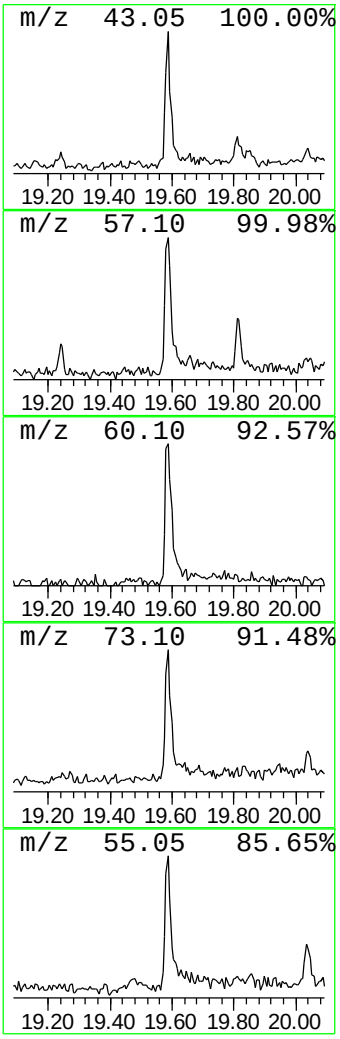
****

Peak Number 6 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.59	2.52 ng	156328	Chrysene-d12	21.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	92
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58





Library Search Compound Report

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Data File : BG042990.D
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Operator : JU
Sample : K5154-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-106S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

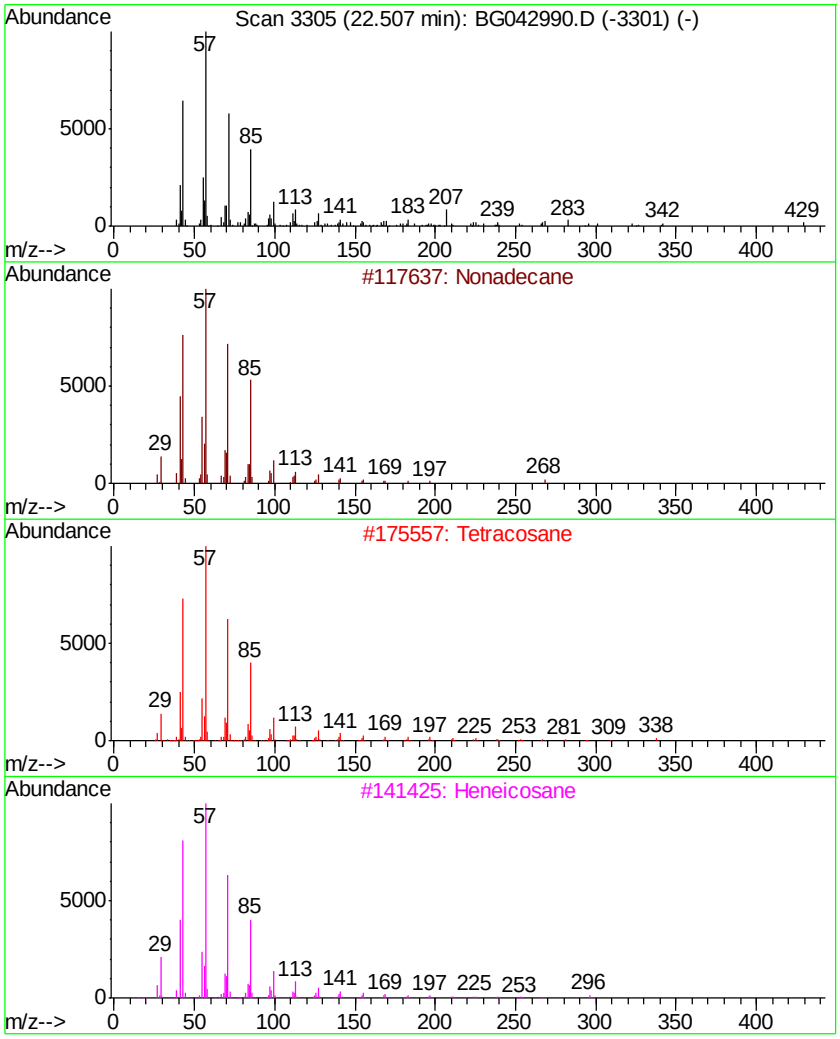
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

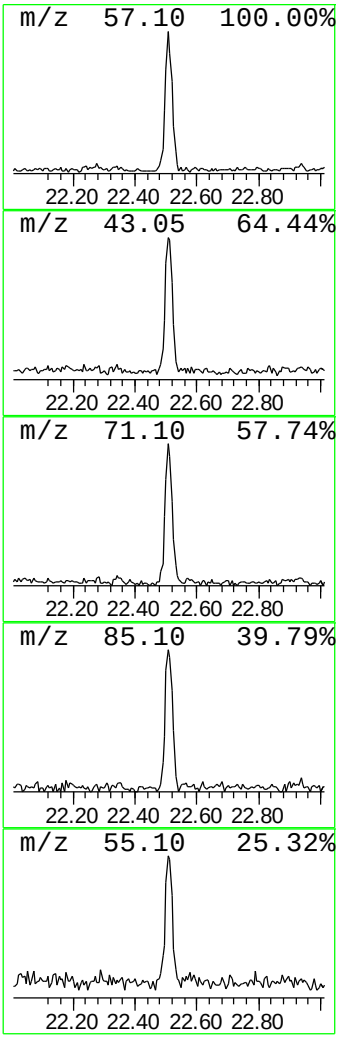
****

Peak Number 7 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.51	2.23 ng	138093	Chrysene-d12	21.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	97
2	Tetracosane	338	C24H50	000646-31-1	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Heptadecane	240	C17H36	000629-78-7	87
5	Octadecane	254	C18H38	000593-45-3	87





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Instrument : BNA_G
ClientSampleId : MW-106S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

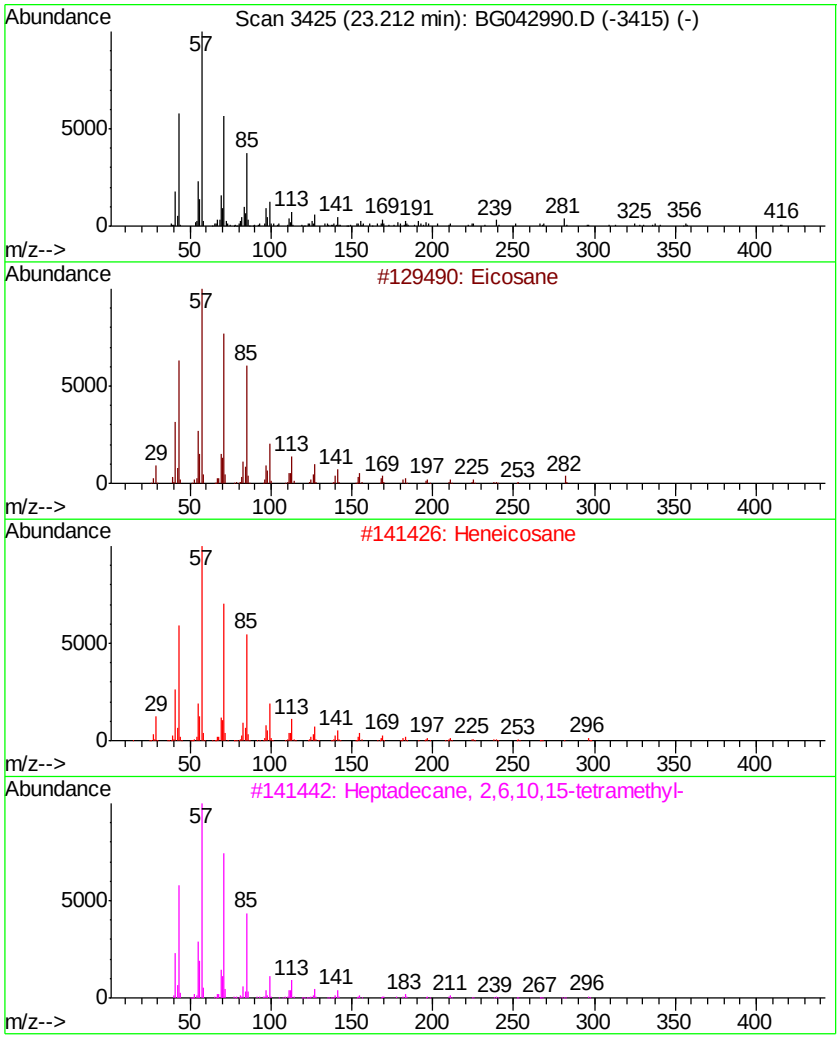
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

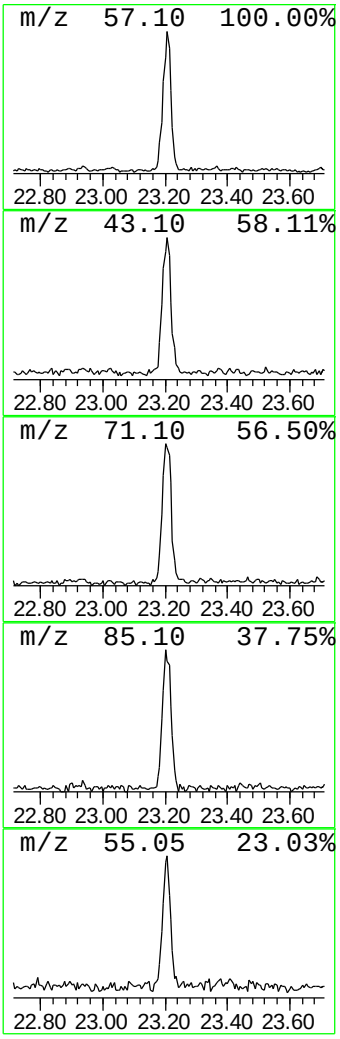
****

Peak Number 8 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.21	4.09 ng	253597	Chrysene-d12	21.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	98
2	Heneicosane	296	C21H44	000629-94-7	97
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	96
4	Hexadecane	226	C16H34	000544-76-3	94
5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	93





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ClientSampleId : MW-106S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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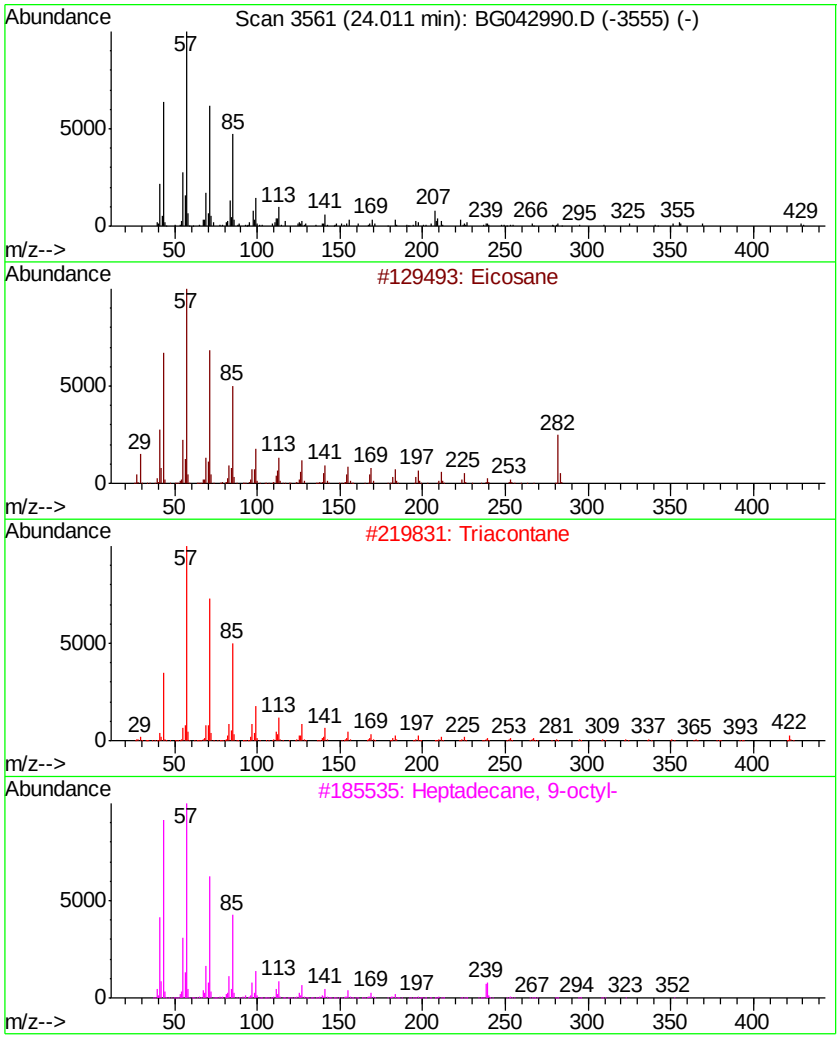
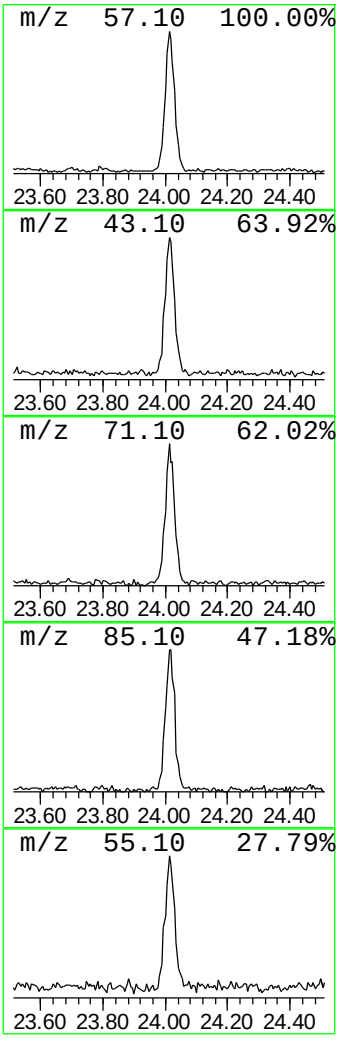
****

Peak Number 9 Triacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.01	3.56 ng	276739	Perylene-d12	24.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Triacontane	422	C30H62	000638-68-6	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Docosane	310	C22H46	000629-97-0	87
5	Octacosane	394	C28H58	000630-02-4	87





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ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-106S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

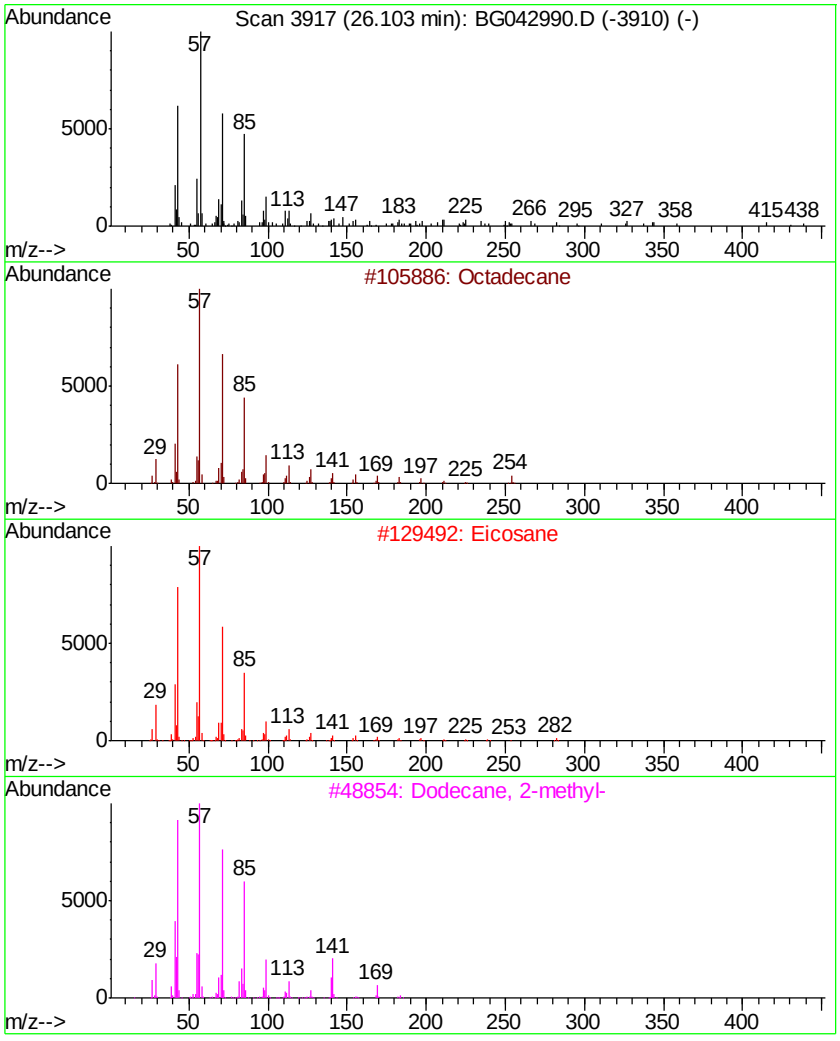
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

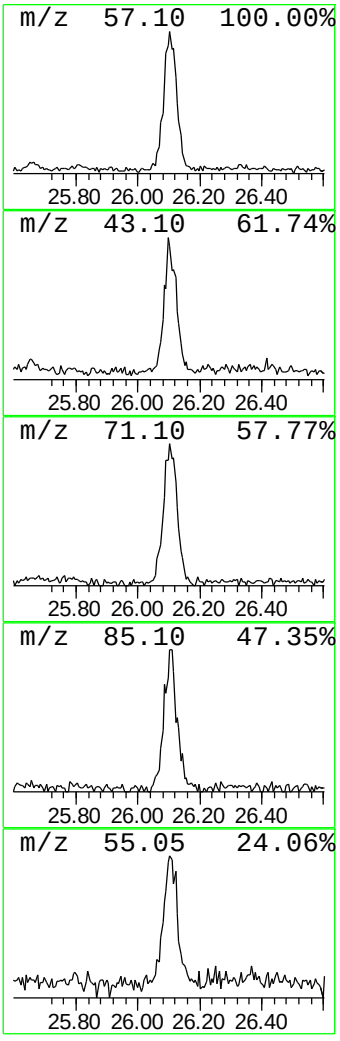
****

Peak Number 10 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.10	2.61 ng	202515	Perylene-d12	24.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Dodecane, 2-methyl-	184	C13H28	001560-97-0	91
4	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	87
5	Octacosane	394	C28H58	000630-02-4	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG100219\
Data File : BG042990.D
Acq On : 2 Oct 2019 18:27
Operator : JU
Sample : K5154-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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
1-Pentene, 2-methyl-	3.18	31.4	ng	707637	1	8.07	451069	20.0
Butane, 2-methoxy...	3.26	33.4	ng	752456	1	8.07	451069	20.0
unknown7.61	7.61	99.4	ng	2241730	1	8.07	451069	20.0
n-Hexadecanoic acid	18.32	5.5	ng	287888	4	17.43	1054950	20.0
Octadecanoic acid	19.59	2.5	ng	156328	5	21.70	1239740	20.0
Nonadecane	22.51	2.2	ng	138093	5	21.70	1239740	20.0
Eicosane	23.21	4.1	ng	253597	5	21.70	1239740	20.0
Triacontane	24.01	3.6	ng	276739	6	24.92	1553100	20.0
Octadecane	26.10	2.6	ng	202515	6	24.92	1553100	20.0