LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG030519\
Data File : BG039780.D
Acq On : 6 Mar 2019 1:22
Operator : JU/SJ
Sample : K1727-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-9

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	3.212	15	21	29	rBV	166257	321779	9.18%	1.882%
2	3.282	29	33	40	rVB	117568	165421	4.72%	0.968%
3	5.696	437	444	455	rVB	343635	563409	16.08%	3.295%
4	7.300	709	717	730	rBV	239507	433945	12.38%	2.538%
5	7.682	774	782	793	rBV	647462	1122689	32.03%	6.566%
6	8.158	855	863	873	rBV	154772	264088	7.54%	1.545%
7	8.481	909	918	926	rBV	540868	946959	27.02%	5.539%
8	9.333	1055	1063	1071	rBV	514984	922564	26.32%	5.396%
9	10.978	1335	1343	1350	rBV	223620	404465	11.54%	2.366%
10	13.404	1748	1756	1764	rBV	1486264	2302232	65.69%	13.465%
11	14.220	1889	1895	1902	rBV	37458	57229	1.63%	0.335%
12	14.784	1984	1991	1999	rVB2	376116	626469	17.88%	3.664%
13	16.265	2237	2243	2257	rBV	1222961	1877900	53.58%	10.984%
14	17.528	2450	2458	2470	rVB	537926	804759	22.96%	4.707%
15	18.373	2595	2602	2614	rBV	86371	152466	4.35%	0.892%
16	19.642	2813	2818	2826	rBV2	47792	81356	2.32%	0.476%
17	20.118	2893	2899	2905	rBV	2568909	3504685	100.00%	20.498%
18	21.405	3114	3118	3132	rBV3	48407	107486	3.07%	0.629%
19	21.816	3181	3188	3196	rVB	523295	877939	25.05%	5.135%
20	21.963	3208	3213	3219	rBV	39615	56383	1.61%	0.330%
21	22.585	3314	3319	3326	rVB2	51091	84936	2.42%	0.497%
22	23.302	3434	3441	3454	rVB	63880	128228	3.66%	0.750%
23	24.142	3576	3584	3590	rBV2	63559	133419	3.81%	0.780%
24	25.182	3743	3761	3775	rVB2	279606	978483	27.92%	5.723%
25	26.304	3943	3952	3965	rVB3	34488	107742	3.07%	0.630%
26	27.720	4186	4193	4206	rVB6	19464	70260	2.00%	0.411%

Sum of corrected areas: 17097291

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Misc :
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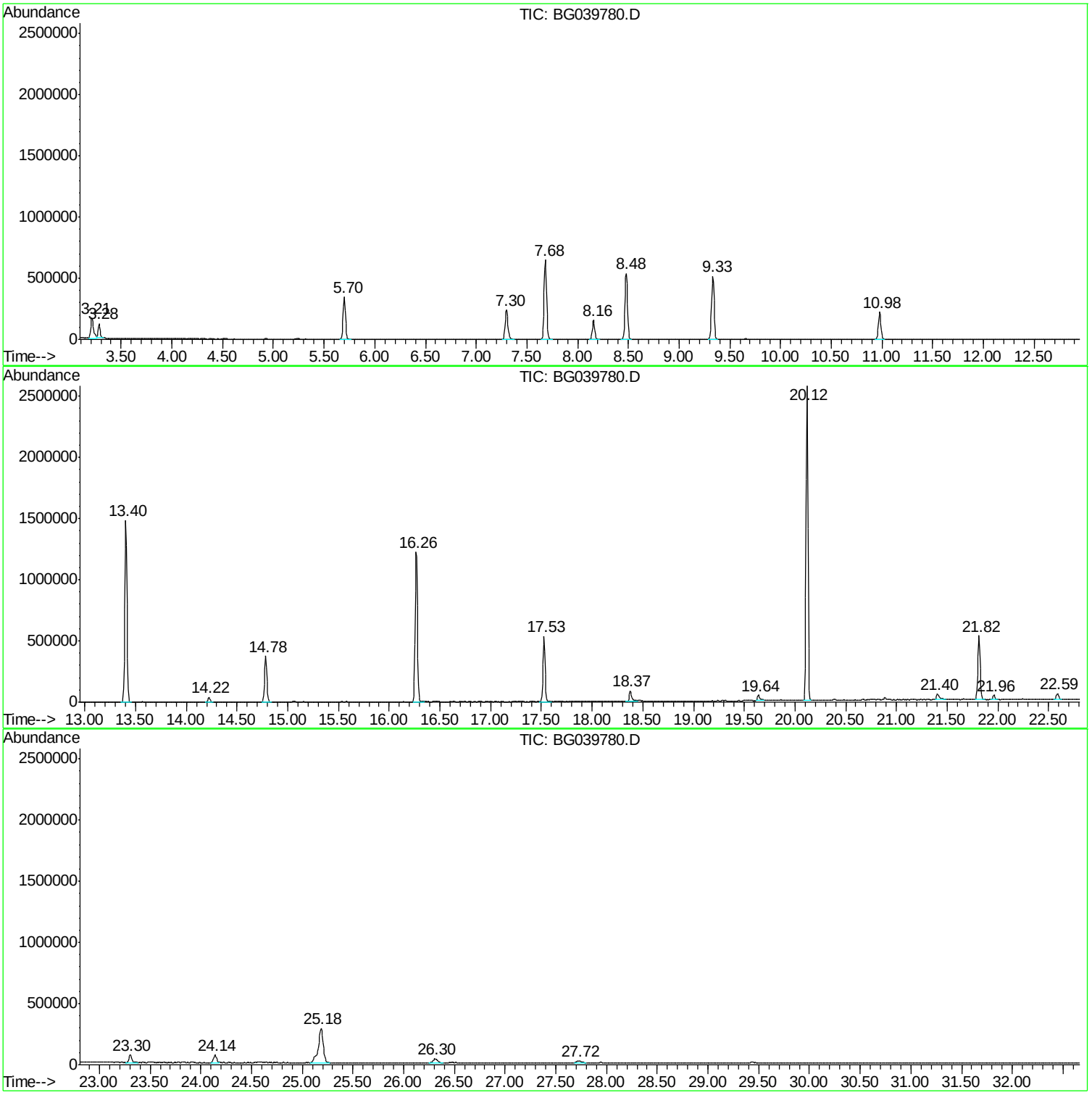
Instrument :
BNA_G
ClientSampleId :
MW-9

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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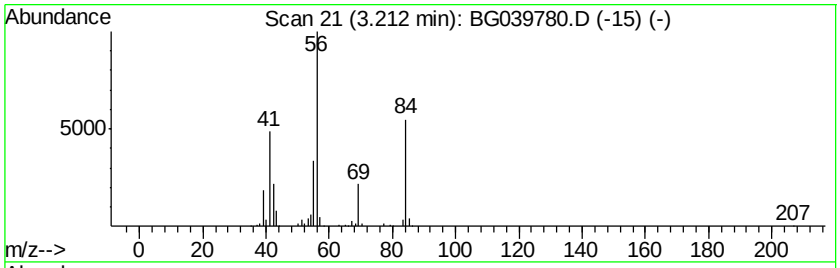
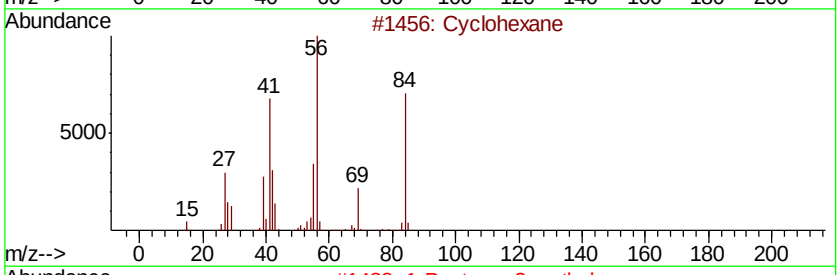
****

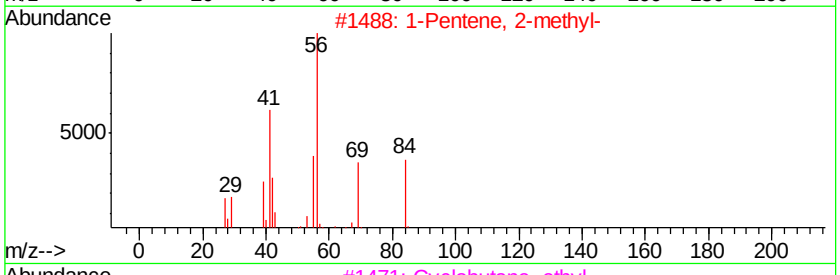
Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 3

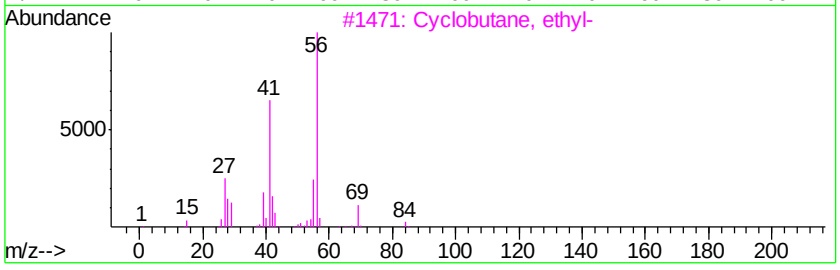
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.21	24.37 ng	321779	1,4-Dichlorobenzene-d4	8.16

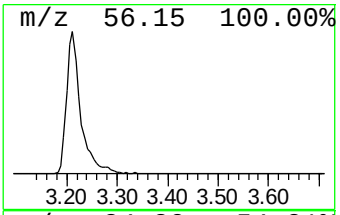
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	91
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	78
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	50
5	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	43

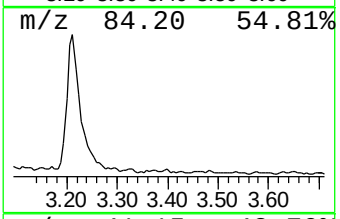


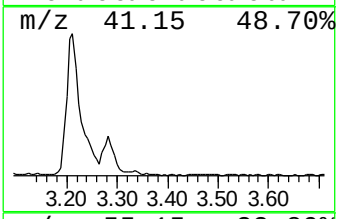


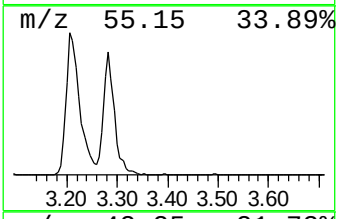


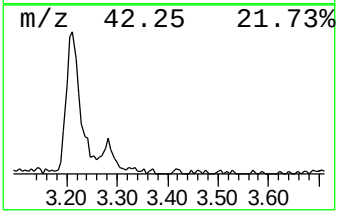












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Instrument : BNA_G
ClientSampleId : MW-9

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

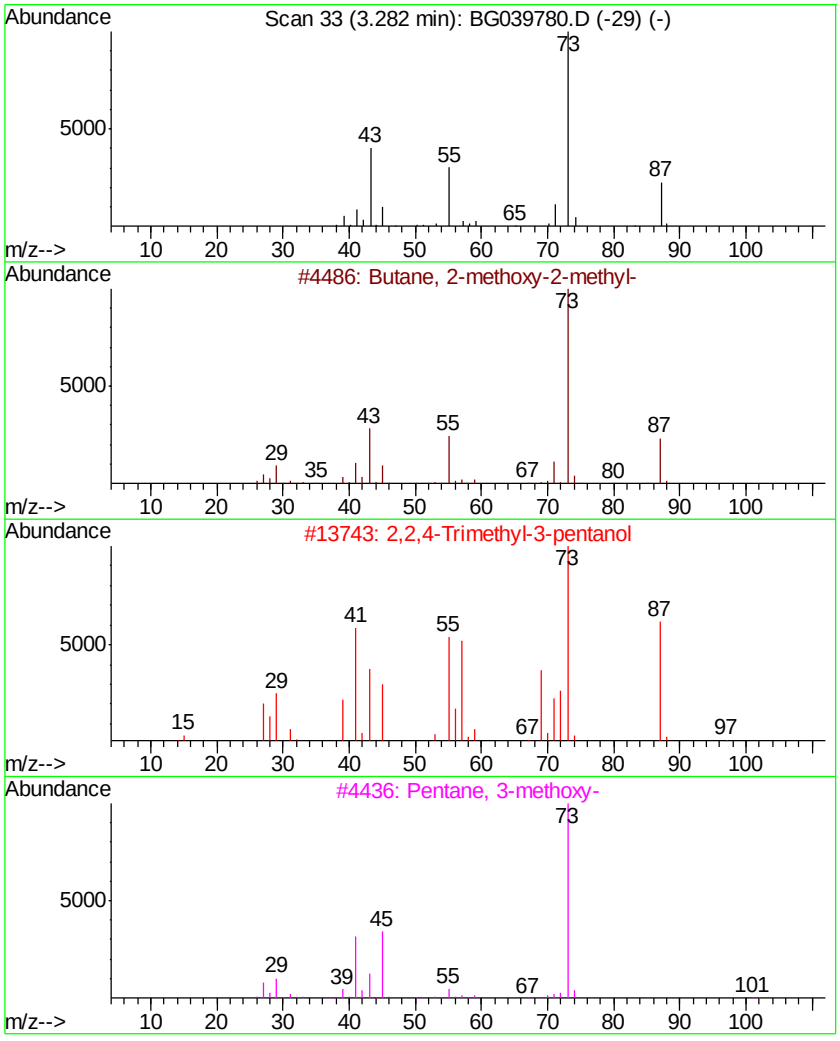
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

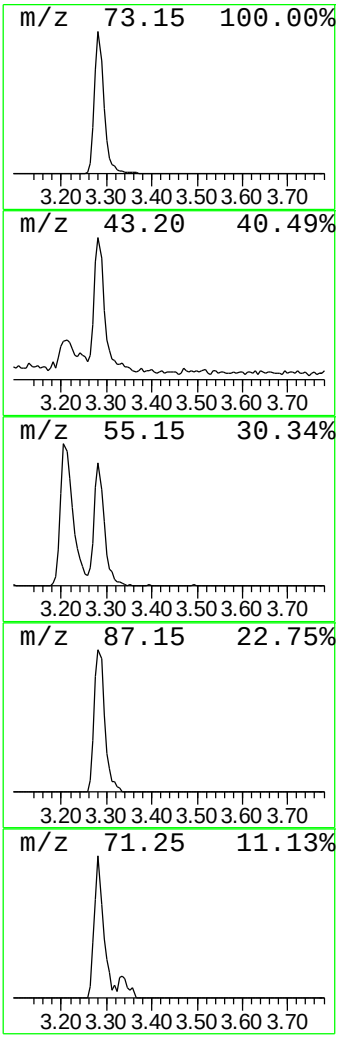
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.28	12.53 ng	165421	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

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Misc :
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Instrument : BNA_G
ClientSampleId : MW-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
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TIC Library : C:\Database\NIST11.L
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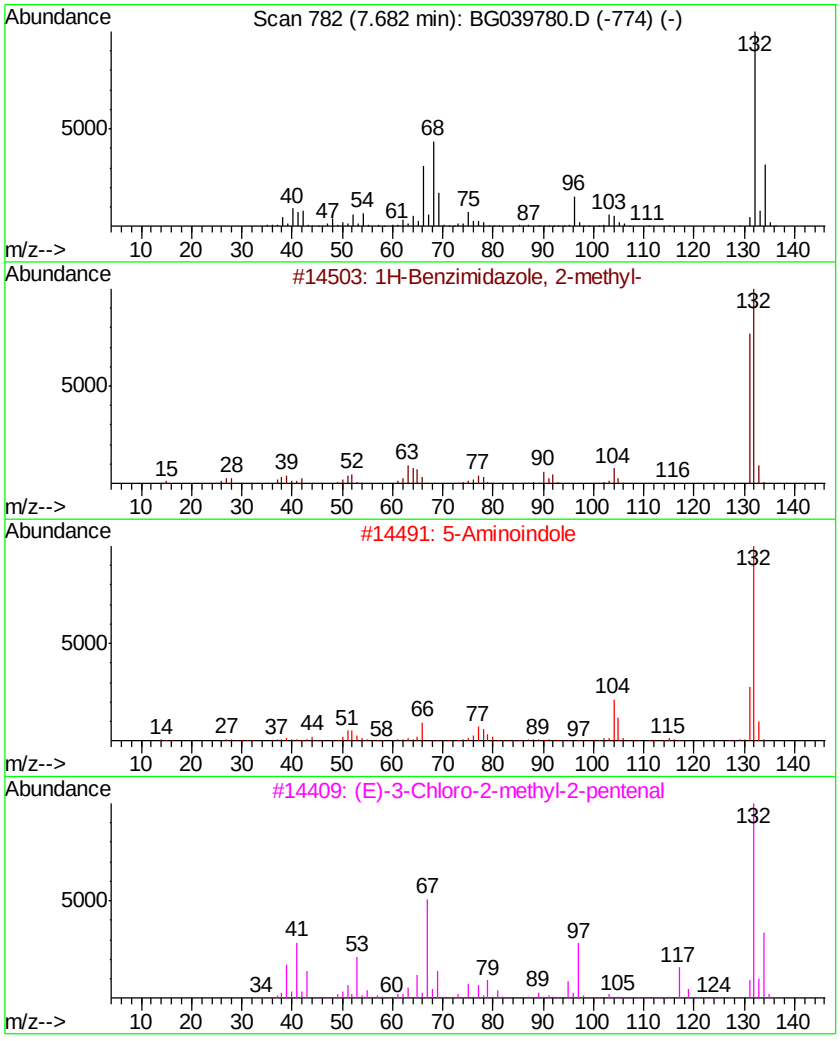
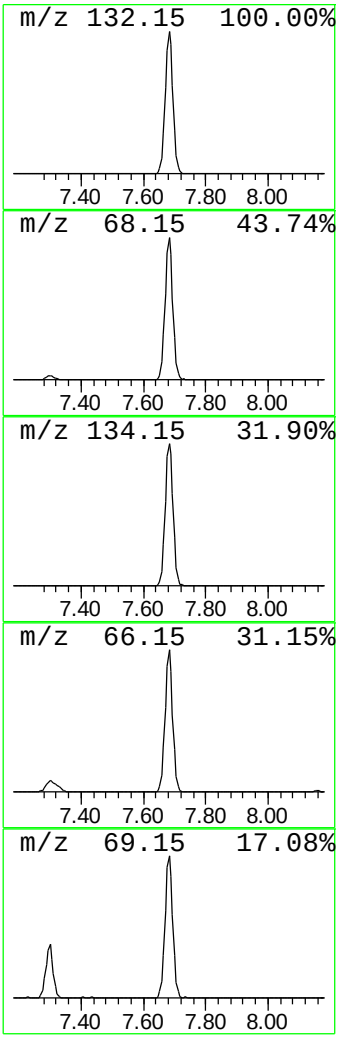
****

Peak Number 3 unknown7.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	85.02 ng	1122690	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2	5-Aminoindole	132	C8H8N2	005192-03-0	22
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





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ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-9

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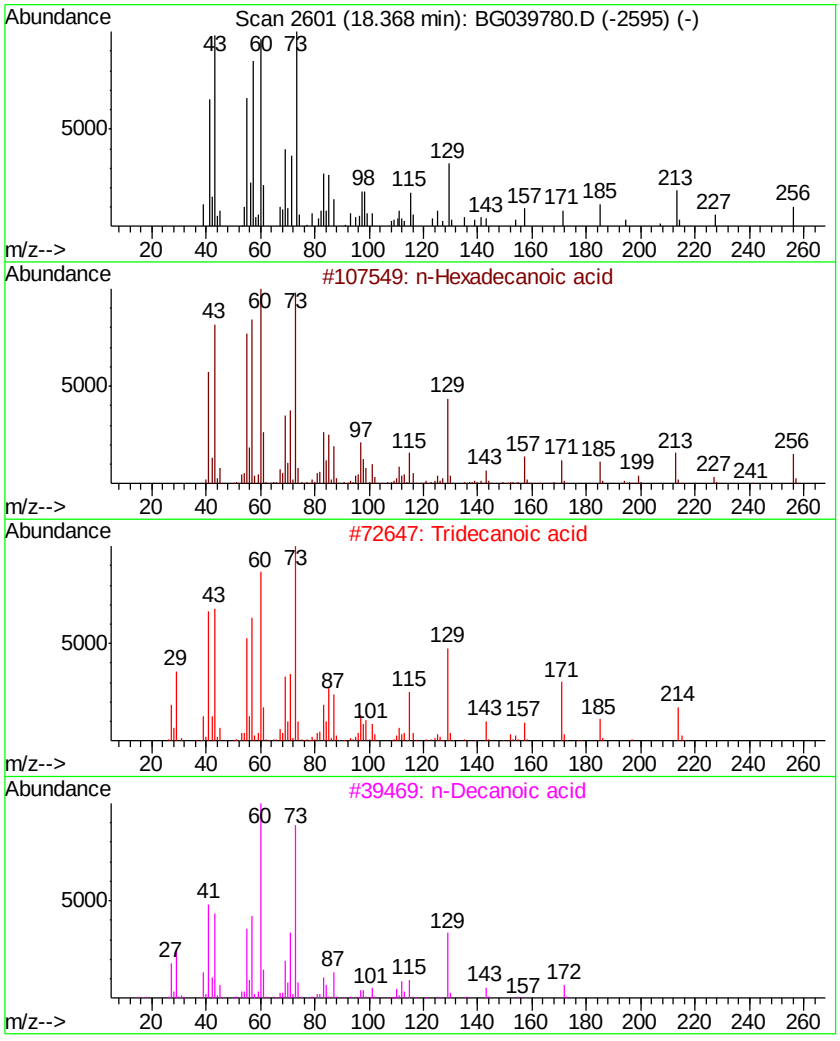
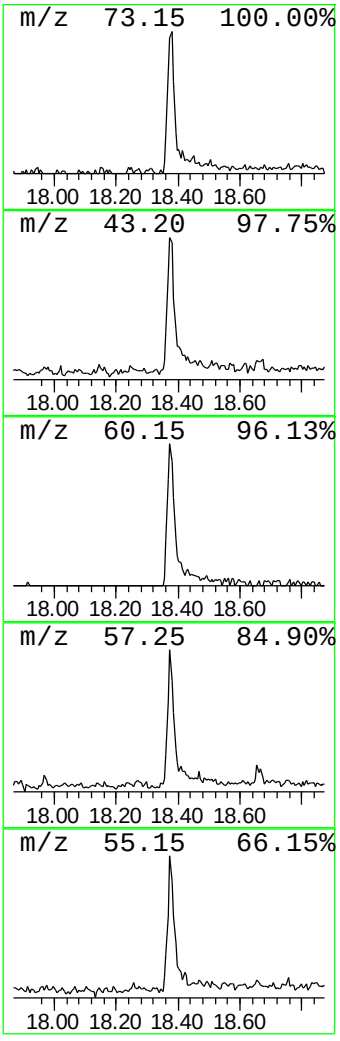
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.37	3.79 ng	152466	Phenanthrene-d10	17.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	n-Decanoic acid	172	C10H20O2	000334-48-5	76
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	18





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Instrument : BNA_G
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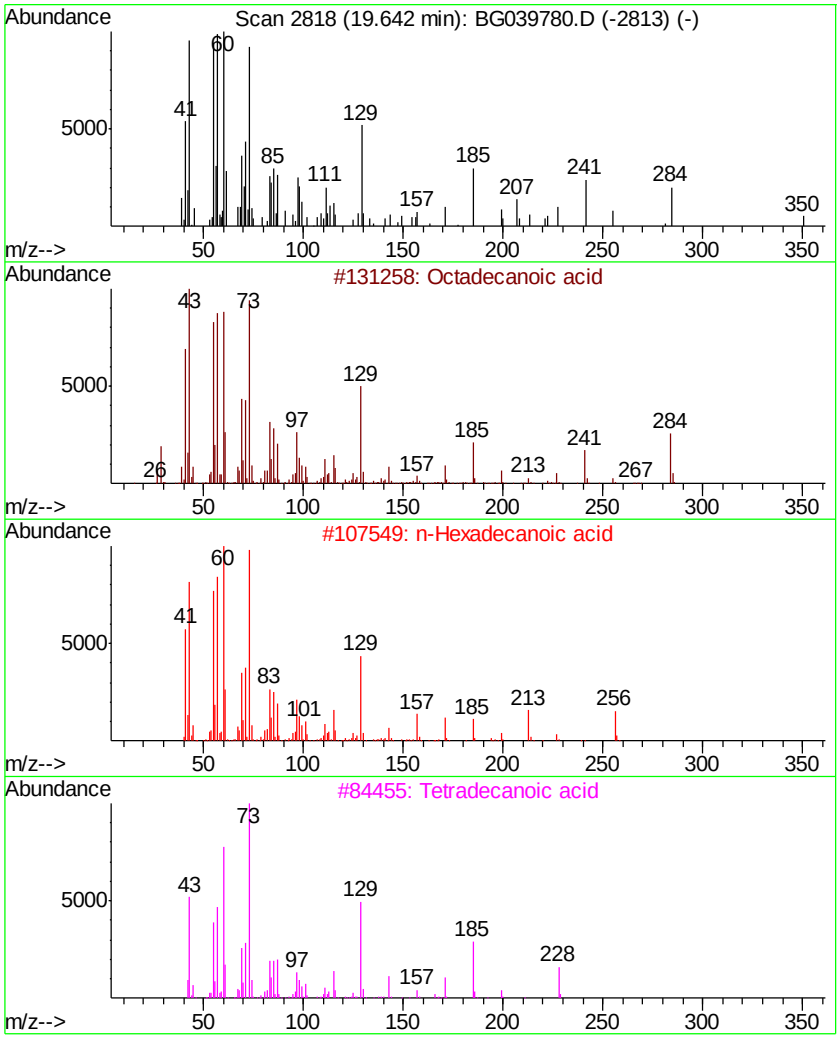
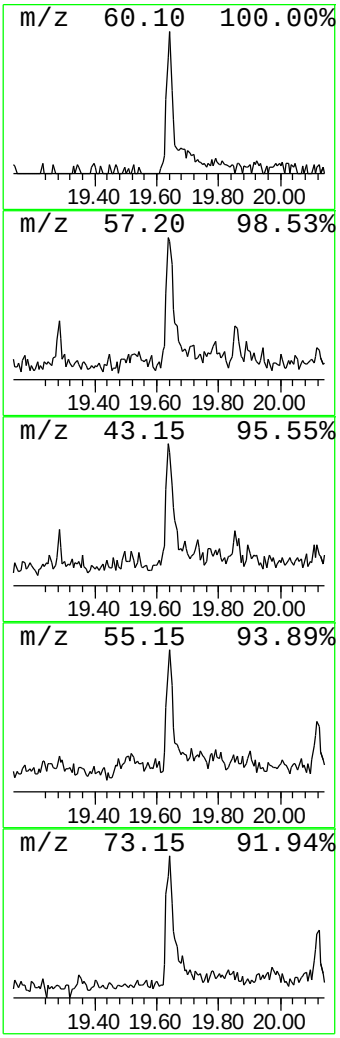
****

Peak Number 6 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.64	2.02 ng	81356	Phenanthrene-d10	17.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	53
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	52





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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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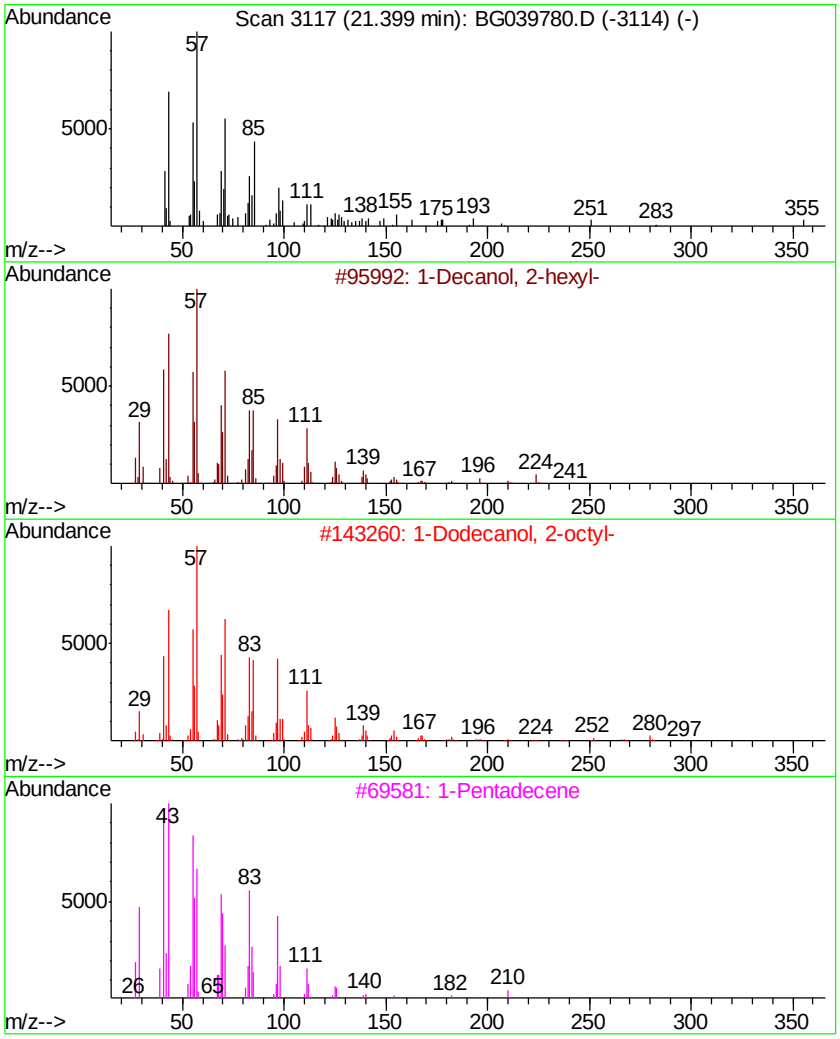
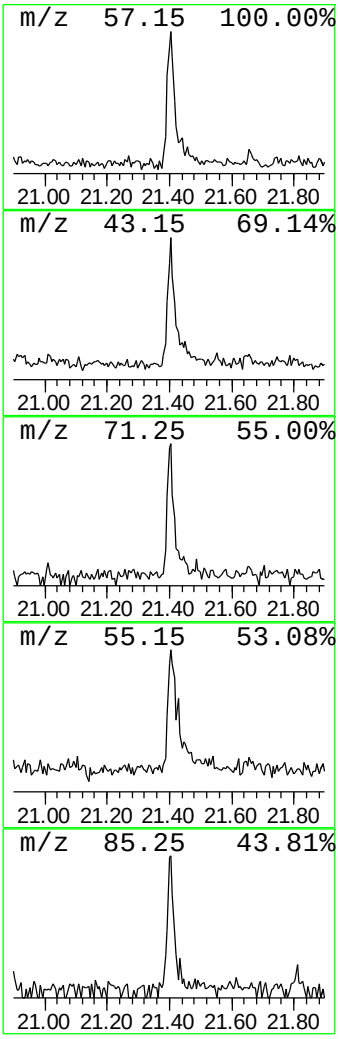
****

Peak Number 7 1-Decanol, 2-hexyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.40	2.45 ng	107486	Chrysene-d12	21.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
2	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
3	1-Pentadecene	210	C15H30	013360-61-7	64
4	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	58
5	Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	53





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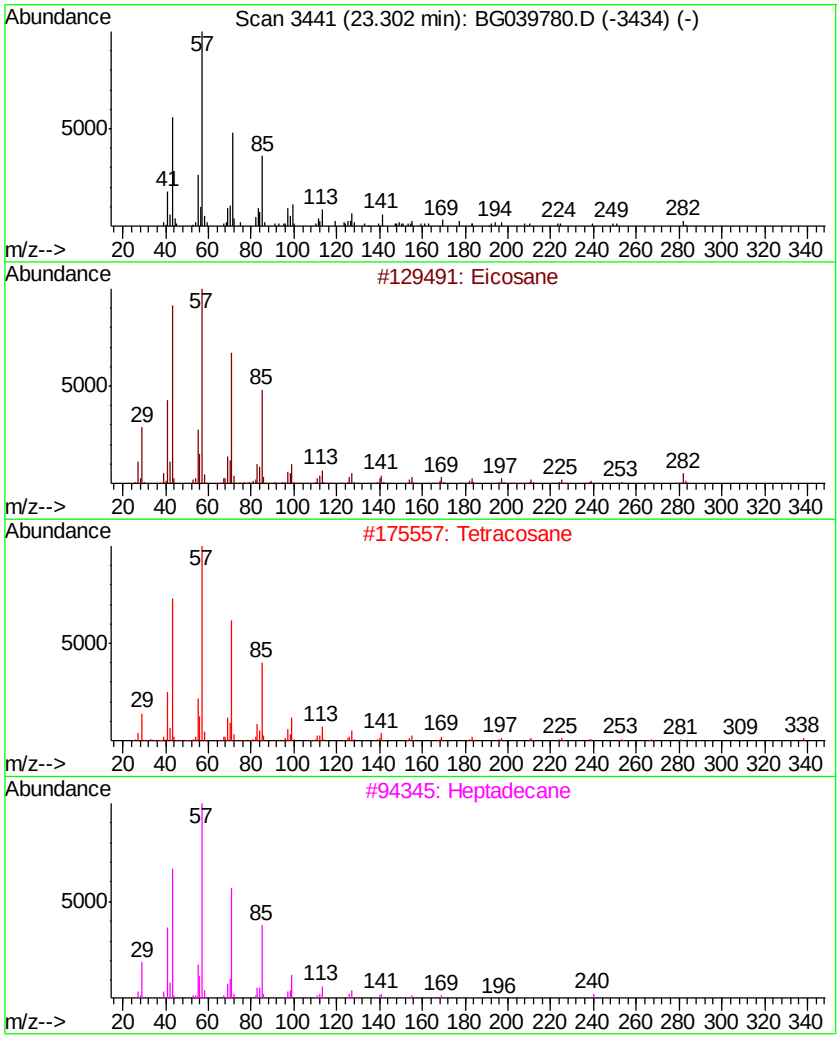
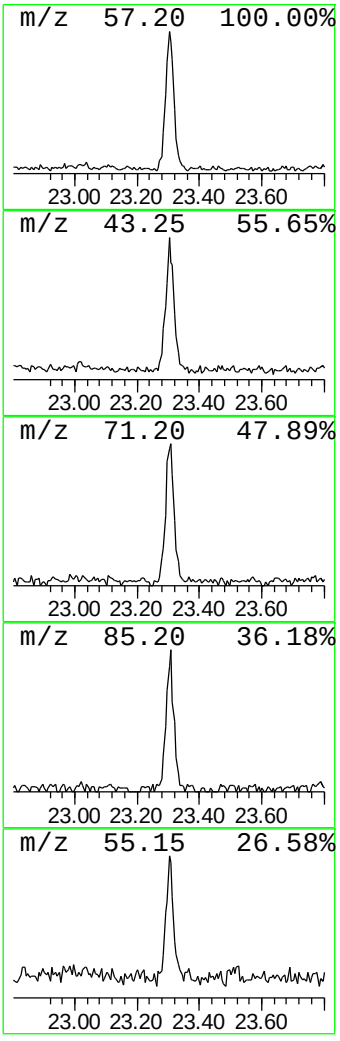
Peak Number 8 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.30	2.92 ng	128228	Chrysene-d12	21.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Tetracosane	338	C24H50	000646-31-1	87
3	Heptadecane	240	C17H36	000629-78-7	83
4	Octacosane	394	C28H58	000630-02-4	83
5	Heneicosane	296	C21H44	000629-94-7	81





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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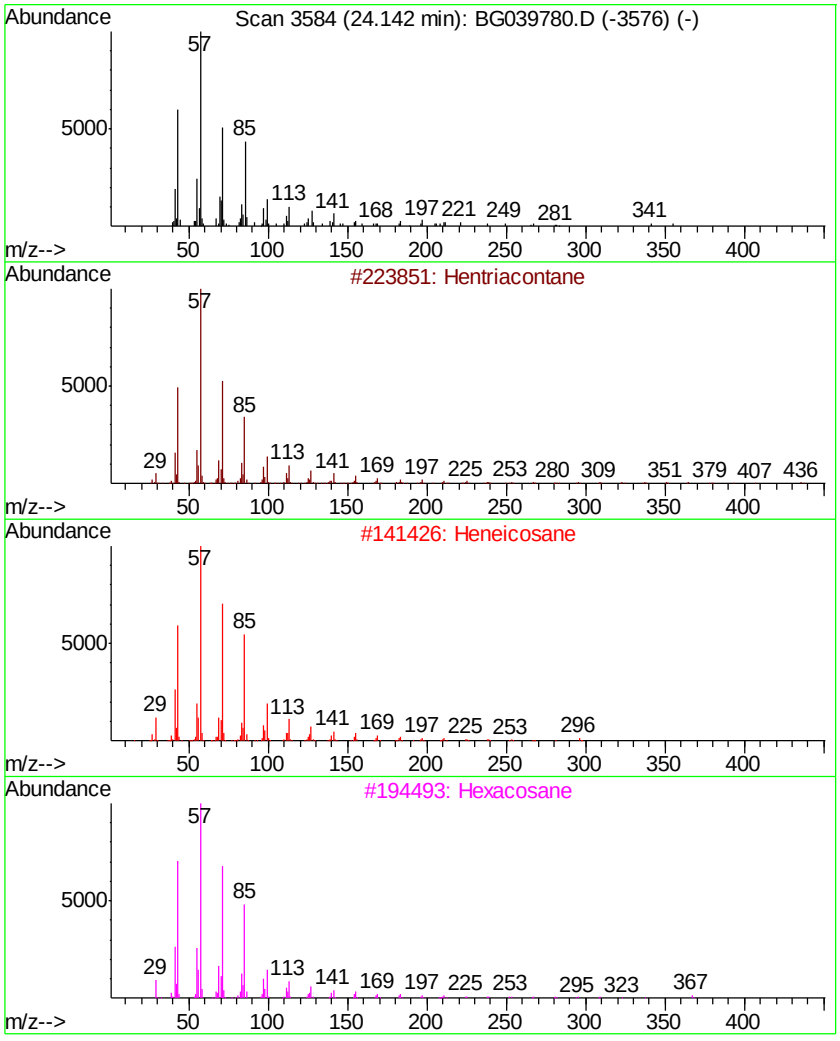
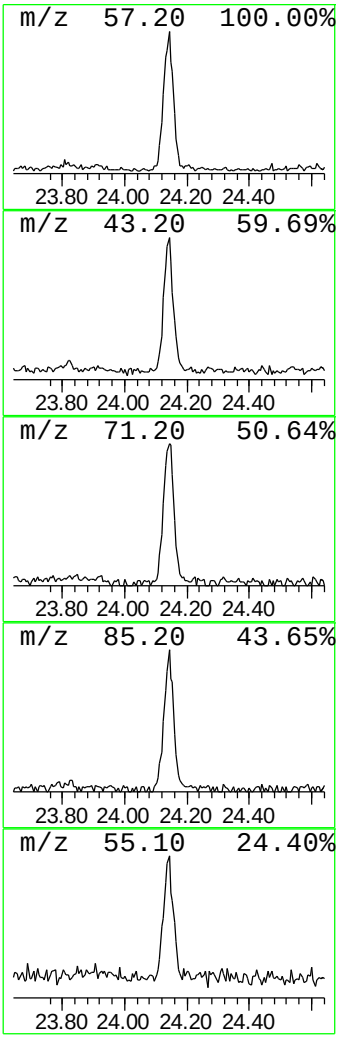
****

Peak Number 9 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.14	2.73 ng	133419	Perylene-d12	25.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Hexacosane	366	C26H54	000630-01-3	87
4	Octacosane	394	C28H58	000630-02-4	87
5	2-methyloctacosane	408	C29H60	1000376-72-8	87





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

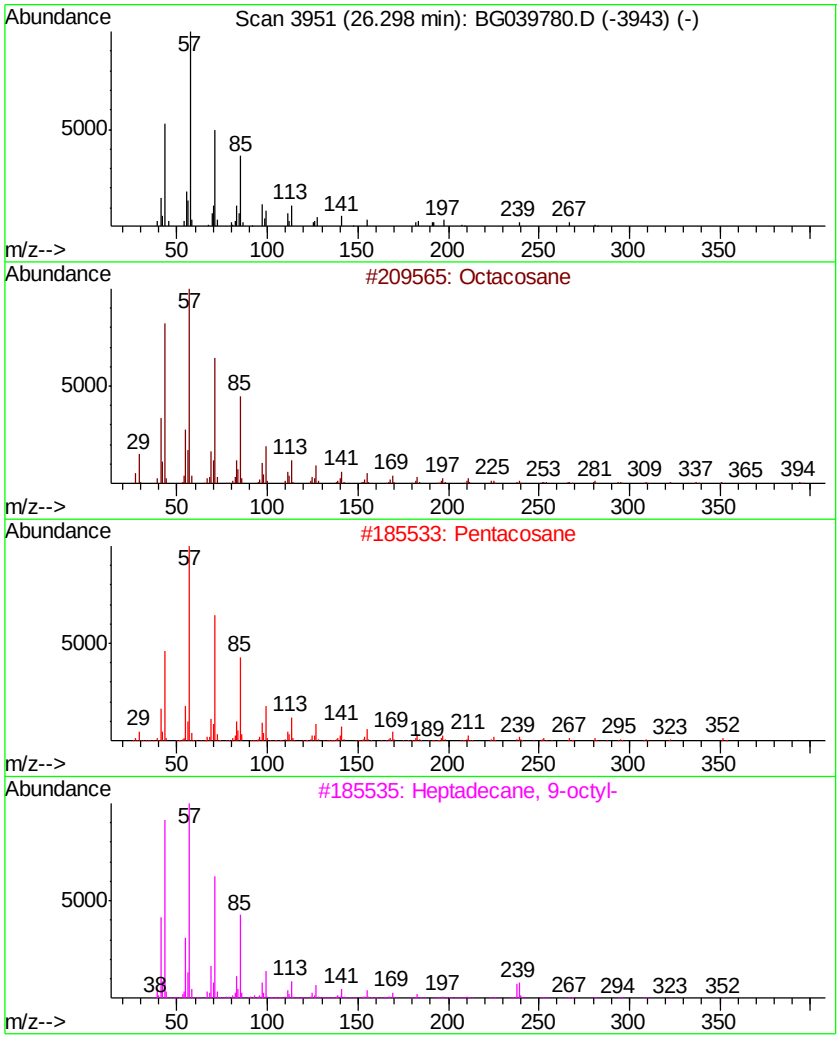
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

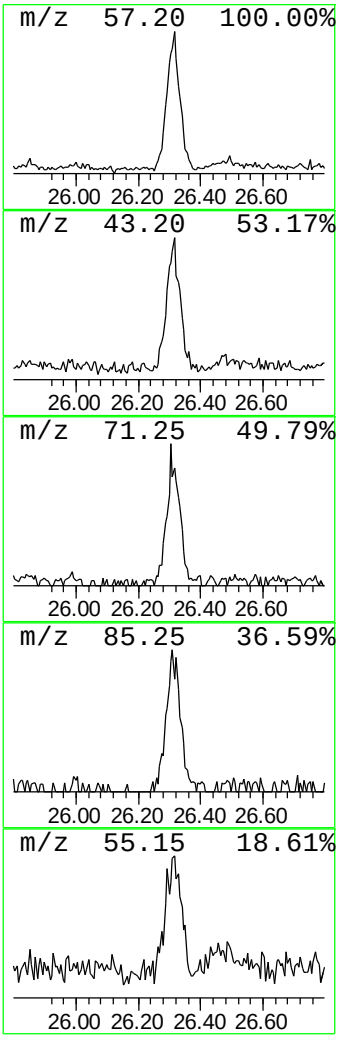
****

Peak Number 10 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.30	2.20 ng	107742	Perylene-d12	25.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Pentacosane	352	C25H52	000629-99-2	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Triacontane	422	C30H62	000638-68-6	87
5	Tetracosane	338	C24H50	000646-31-1	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG030519\
Data File : BG039780.D
Acq On : 6 Mar 2019 1:22
Operator : JU/SJ
Sample : K1727-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-9

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
1-Pentene, 2-methyl-	3.21	24.4	ng	321779	1	8.16	264088	20.0
Butane, 2-methoxy...	3.28	12.5	ng	165421	1	8.16	264088	20.0
unknown7.68	7.68	85.0	ng	1122690	1	8.16	264088	20.0
n-Hexadecanoic acid	18.37	3.8	ng	152466	4	17.53	804759	20.0
Octadecanoic acid	19.64	2.0	ng	81356	4	17.53	804759	20.0
1-Decanol, 2-hexyl-	21.40	2.5	ng	107486	5	21.82	877939	20.0
Eicosane	23.30	2.9	ng	128228	5	21.82	877939	20.0
Hentriacontane	24.14	2.7	ng	133419	6	25.18	978483	20.0
Octacosane	26.30	2.2	ng	107742	6	25.18	978483	20.0