

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011719\
 Data File : BG039191.D
 Acq On : 17 Jan 2019 18:01
 Operator : JU/SJ
 Sample : K1139-21
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 T-CONTAINMENT

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BG010919.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	3.132	3	7	13	rVB	27251	37377	5.46%	0.827%
2	5.571	416	422	431	rBV	16784	27772	4.05%	0.615%
3	7.181	690	696	698	rBV2	11300	19614	2.86%	0.434%
4	7.545	752	758	766	rBV	28057	47580	6.95%	1.053%
5	8.015	831	838	849	rVB	66322	120171	17.55%	2.660%
6	8.338	884	893	901	rBB	87626	156856	22.90%	3.471%
7	9.190	1030	1038	1051	rBV	86684	167034	24.39%	3.697%
8	10.829	1310	1317	1327	rVB	94170	179053	26.14%	3.963%
9	13.273	1723	1733	1744	rBV	279590	447309	65.31%	9.900%
10	13.514	1768	1774	1781	rBV3	18205	27684	4.04%	0.613%
11	14.102	1868	1874	1887	rVB	124453	187614	27.39%	4.152%
12	14.654	1962	1968	1978	rVB2	179930	301599	44.03%	6.675%
13	16.146	2215	2222	2232	rBV4	65793	106833	15.60%	2.364%
14	16.340	2246	2255	2258	rBV6	6564	14498	2.12%	0.321%
15	17.157	2390	2394	2399	rBV2	14217	22436	3.28%	0.497%
16	17.404	2429	2436	2443	rBV2	237822	386601	56.44%	8.556%
17	17.762	2495	2497	2503	rBV7	8421	11605	1.69%	0.257%
18	18.267	2579	2583	2586	rBV4	18409	27542	4.02%	0.610%
19	18.491	2617	2621	2625	rBV7	7780	12667	1.85%	0.280%
20	18.696	2654	2656	2659	rBV4	10282	7098	1.04%	0.157%
21	18.931	2695	2696	2699	rBV3	8785	10041	1.47%	0.222%
22	18.990	2704	2706	2710	rVV4	12183	13685	2.00%	0.303%
23	19.290	2755	2757	2759	rBV3	13132	11230	1.64%	0.249%
24	20.007	2873	2879	2886	rBV	531393	684918	100.00%	15.158%
25	20.911	3030	3033	3035	rBV3	9592	13488	1.97%	0.299%
26	21.276	3091	3095	3105	rVB2	57825	99441	14.52%	2.201%
27	21.528	3134	3138	3141	rBV4	5242	7502	1.10%	0.166%
28	21.675	3157	3163	3171	rVB2	242852	418568	61.11%	9.264%
29	21.810	3183	3186	3191	rVB3	11606	16408	2.40%	0.363%
30	22.092	3232	3234	3236	rBV3	10081	11415	1.67%	0.253%
31	22.416	3284	3289	3295	rBV	29050	52592	7.68%	1.164%
32	22.662	3330	3331	3338	rBV7	5502	10903	1.59%	0.241%
33	22.809	3352	3356	3360	rVB6	4989	7047	1.03%	0.156%
34	23.103	3401	3406	3413	rVB2	40085	66293	9.68%	1.467%

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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

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Peak separation: 5

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35	23.303	3433	3440	3448	rVB	40549	87970	12.84%	1.947%
36	23.908	3535	3543	3550	rBV3	34577	72703	10.61%	1.609%
37	24.848	3695	3703	3709	rBV2	28359	76270	11.14%	1.688%
38	24.942	3709	3719	3732	rVB2	156213	453927	66.27%	10.046%
39	25.976	3886	3895	3908	rVB5	16219	53782	7.85%	1.190%
40	27.327	4117	4125	4135	rVB9	8592	27371	4.00%	0.606%
41	28.949	4394	4401	4402	rBV5	4217	6885	1.01%	0.152%
42	32.169	4944	4949	4953	rBV5	3850	7056	1.03%	0.156%

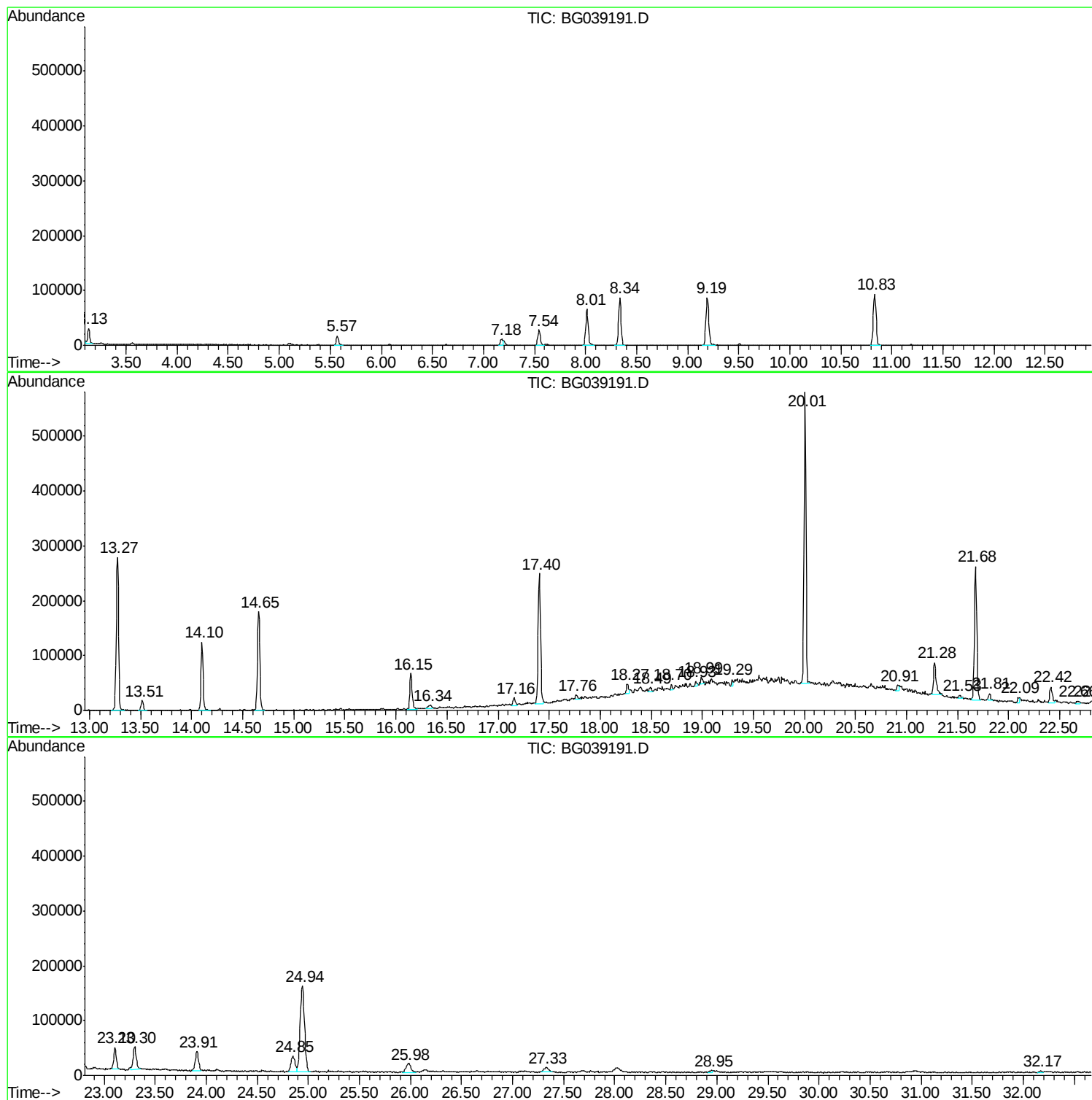
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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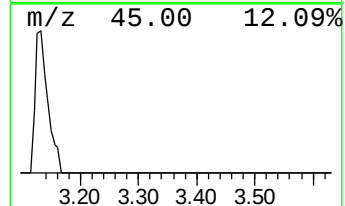
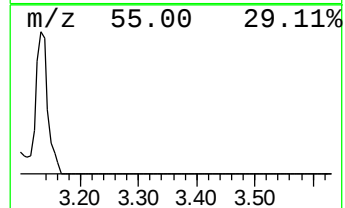
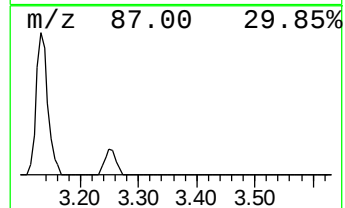
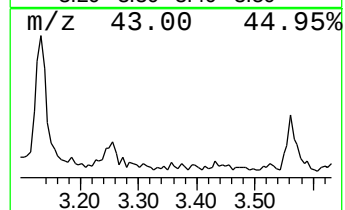
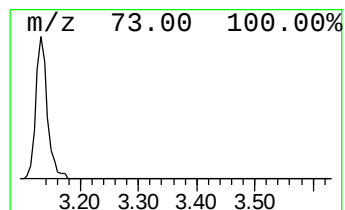
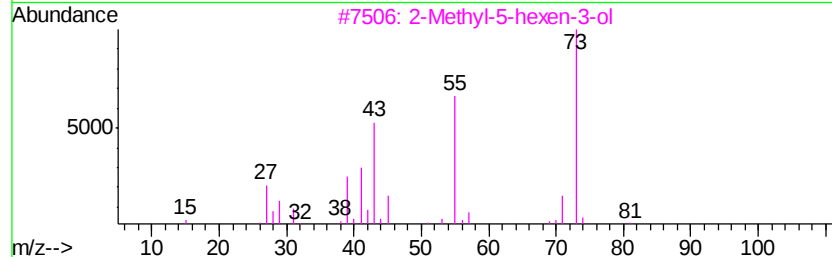
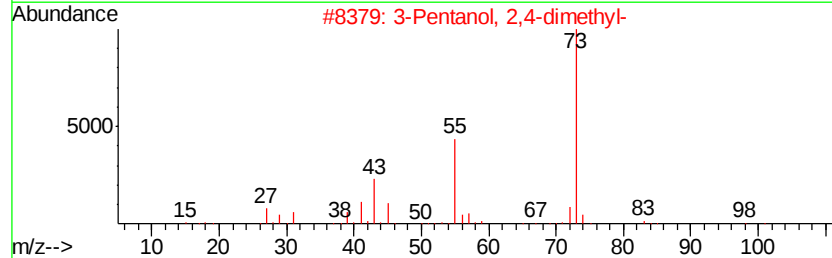
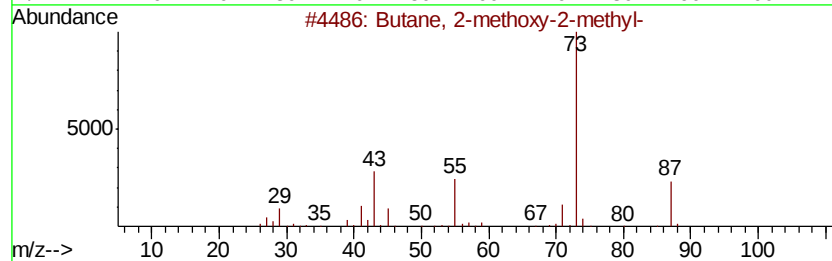
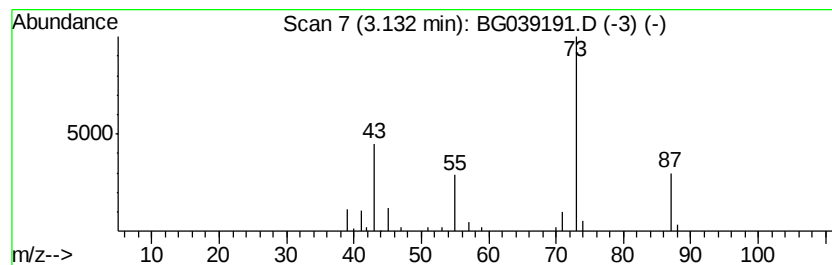
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	6.22 ng	37377	1,4-Dichlorobenzene-d4	8.01

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4			2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	17
5			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9



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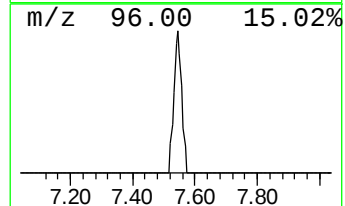
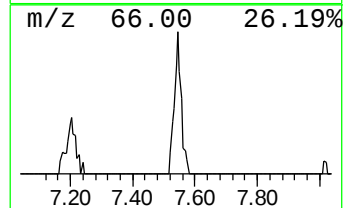
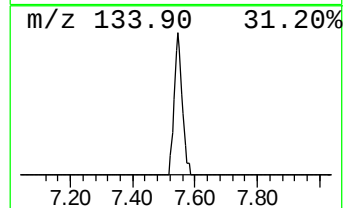
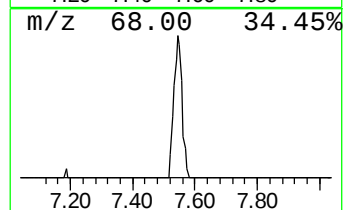
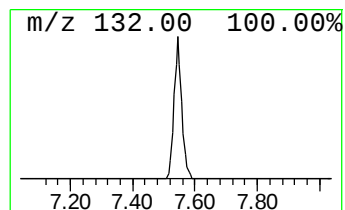
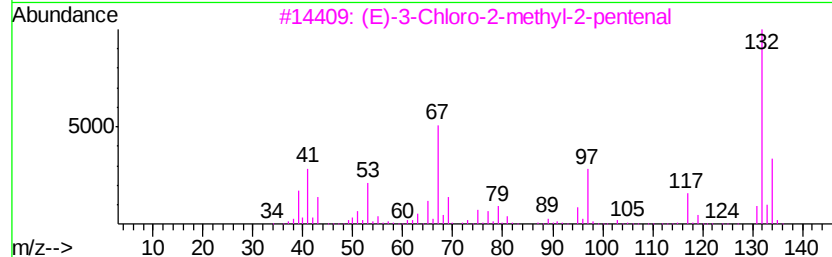
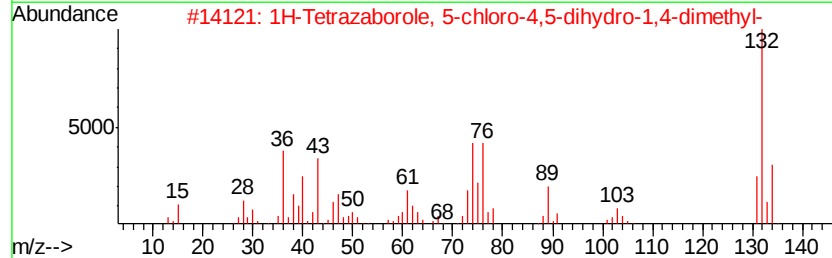
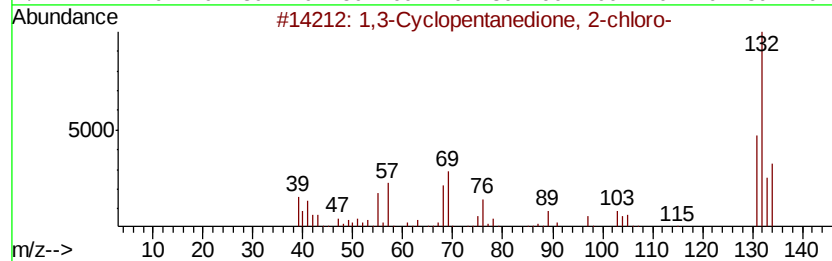
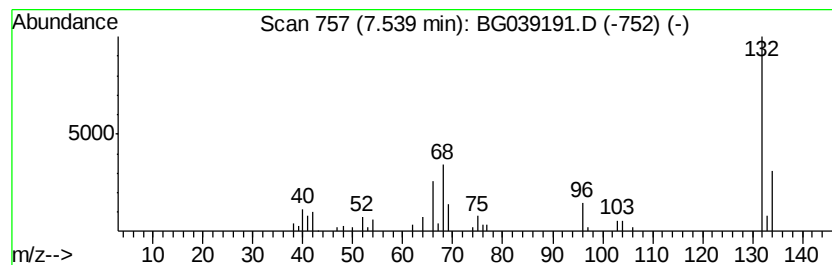
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Peak Number 2 unknown7.54 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	7.92 ng	47580	1,4-Dichlorobenzene-d4	8.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	38
2		1H-Tetrazaborole, 5-chloro-4,5-d...	132	C2H6BClN4	021960-49-6	17
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	16
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12



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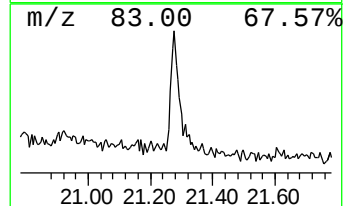
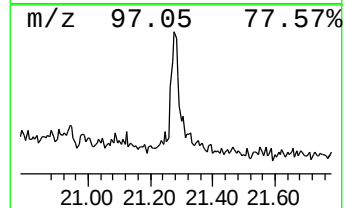
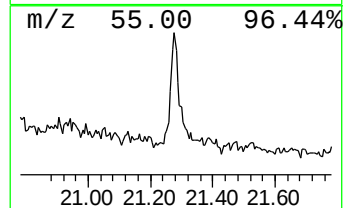
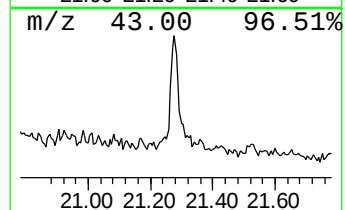
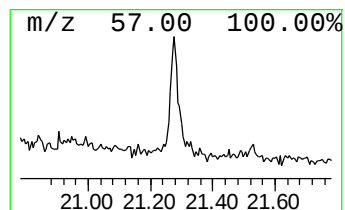
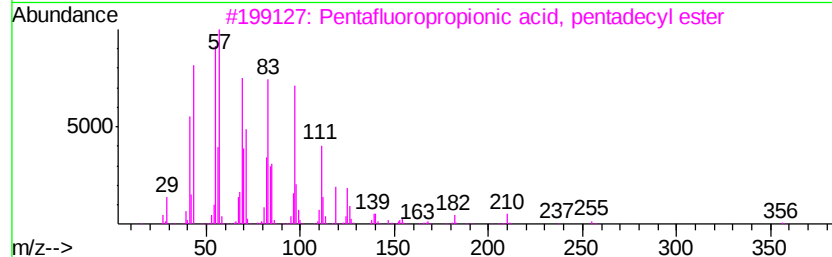
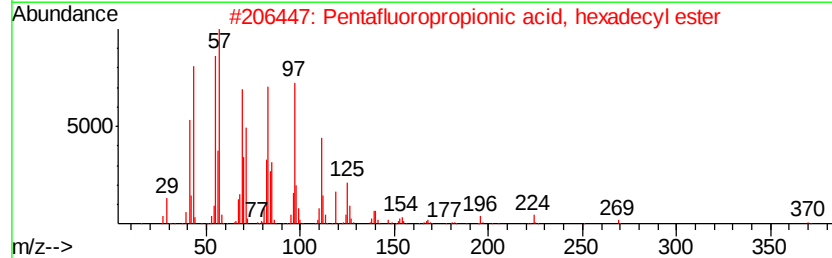
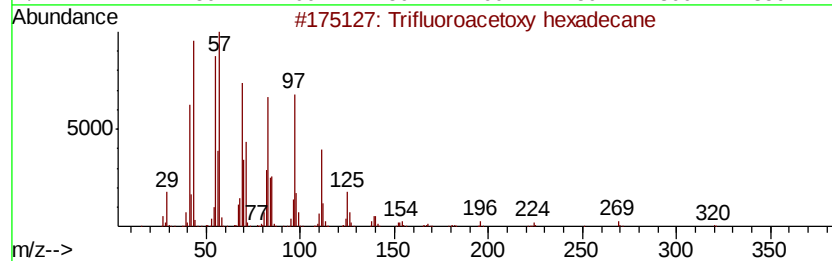
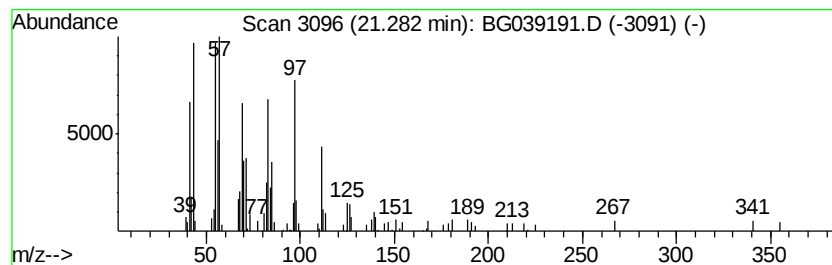
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.28	4.75 ng	99441	Chrysene-d12		21.68	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	95
2		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	95
3		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
4		Heptadecyl heptafluorobutvrate	452	C21H35F7O2	959085-66-6	94
5		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94



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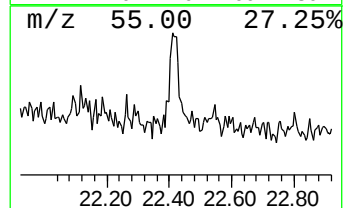
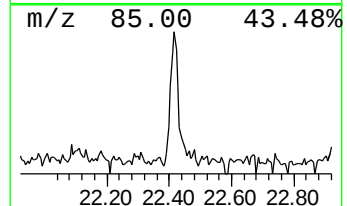
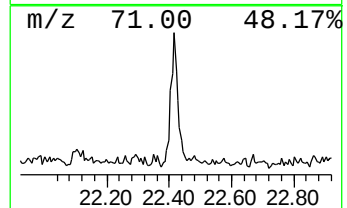
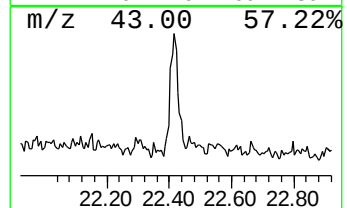
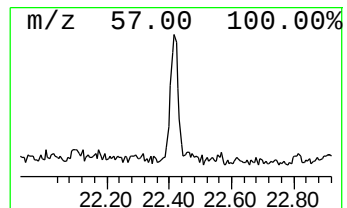
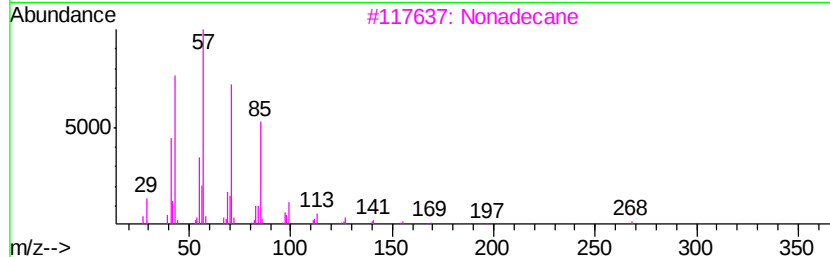
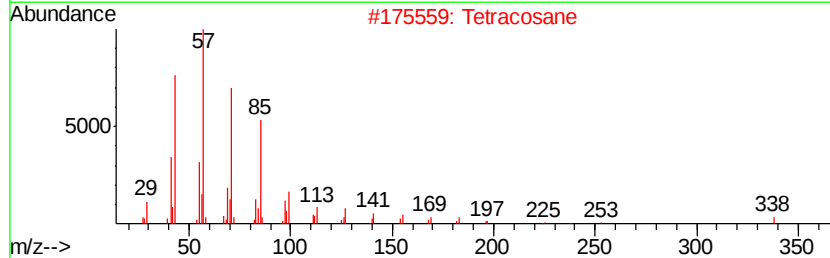
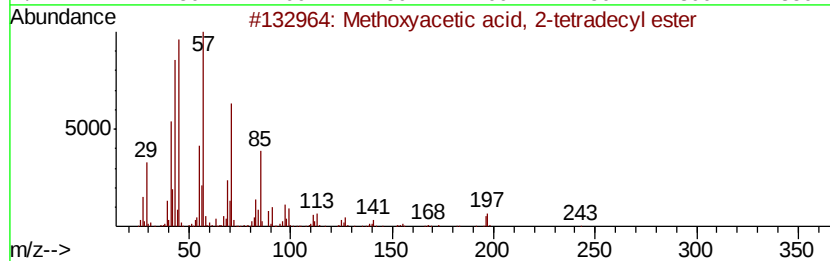
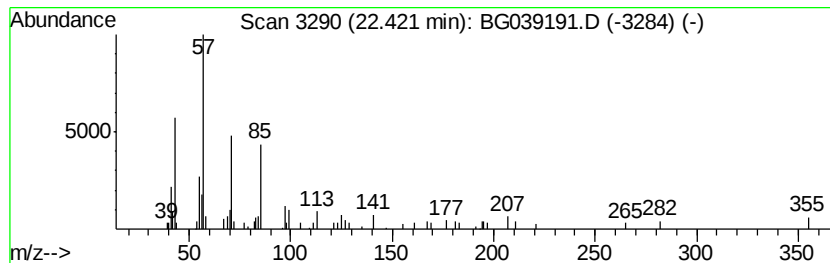
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Peak Number 5 Methoxyacetic acid, 2-tetra... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.42	2.51 ng	52592	Chrysene-d12	21.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methoxvacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	90
2		Tetracosane	338	C24H50	000646-31-1	87
3		Nonadecane	268	C19H40	000629-92-5	87
4		Hexacosane	366	C26H54	000630-01-3	83
5		Heptadecane	240	C17H36	000629-78-7	80



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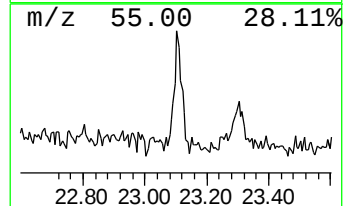
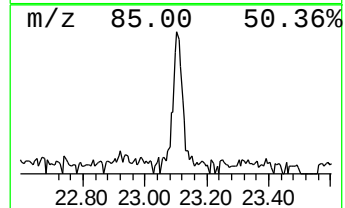
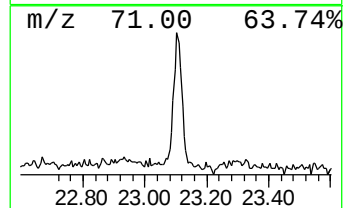
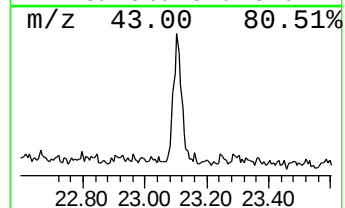
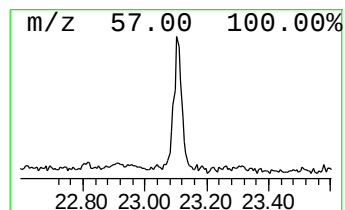
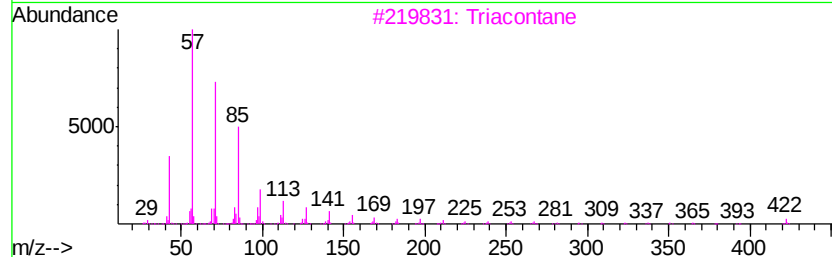
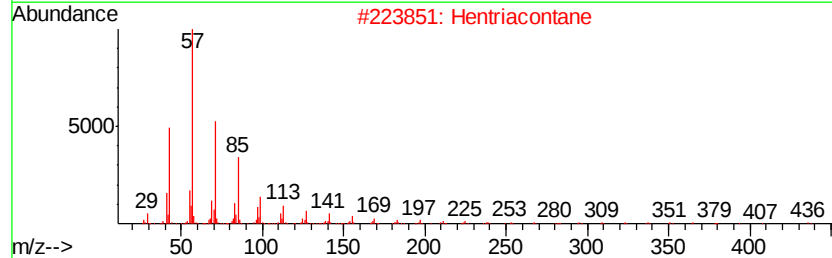
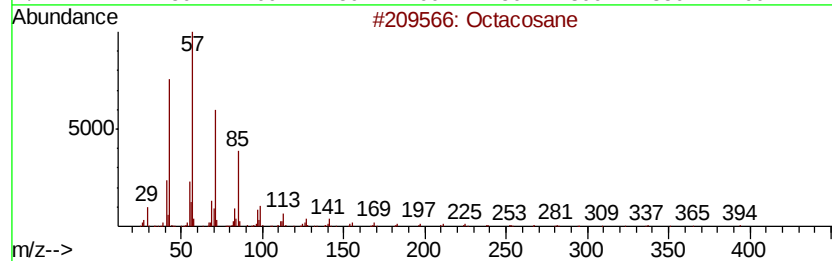
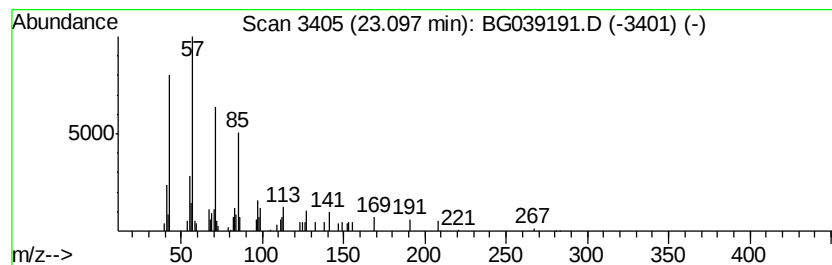
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.10	3.17 ng	66293	Chrysene-d12	21.68

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	87
2	Hentriacontane		437	C31H64	000630-04-6	87
3	Triacontane		422	C30H62	000638-68-6	87
4	Hexatriacontane		507	C36H74	000630-06-8	83
5	Eicosane		282	C20H42	000112-95-8	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011719\
Data File : BG039191.D
Acq On : 17 Jan 2019 18:01
Operator : JU/SJ
Sample : K1139-21
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
T-CONTAINMENT

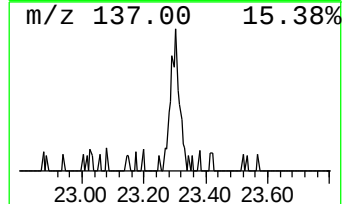
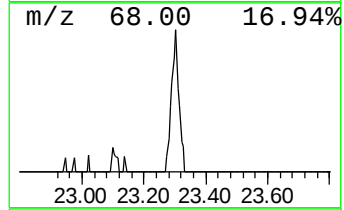
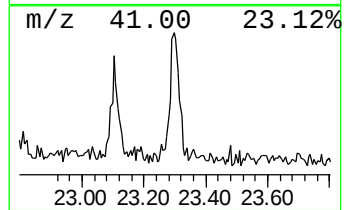
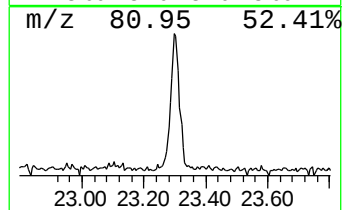
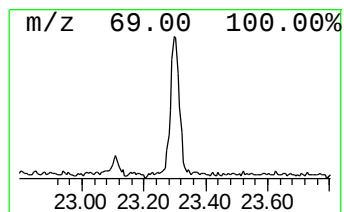
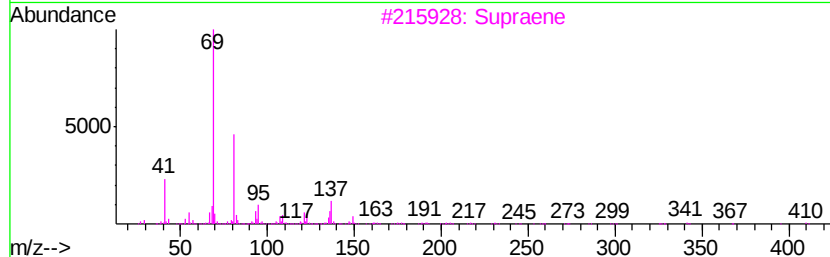
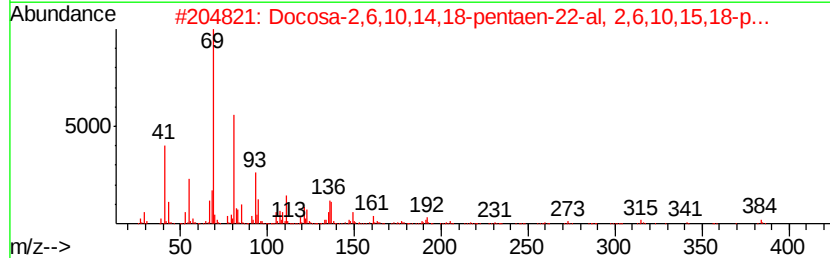
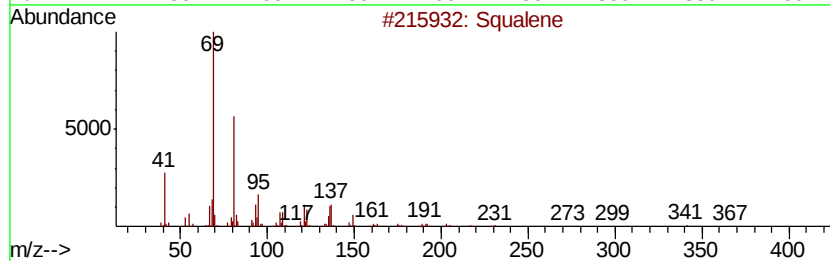
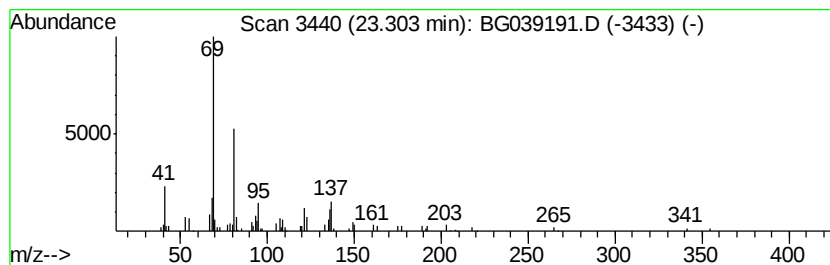
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.30	4.20 ng	87970	Chrysene-d12	21.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	91
3		Supraene	410	C30H50	007683-64-9	90
4		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	78
5		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011719\
Data File : BG039191.D
Acq On : 17 Jan 2019 18:01
Operator : JU/SJ
Sample : K1139-21
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
T-CONTAINMENT

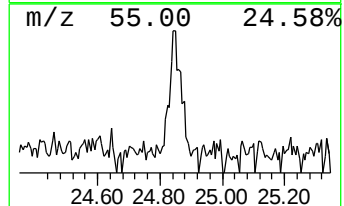
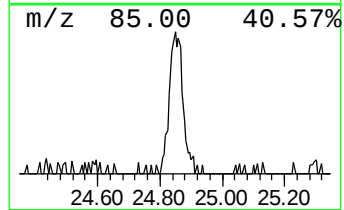
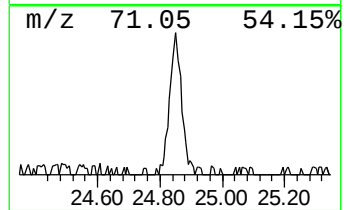
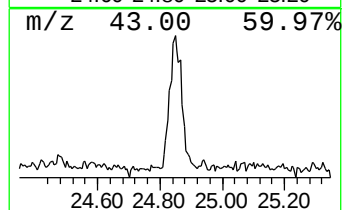
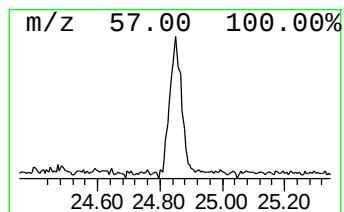
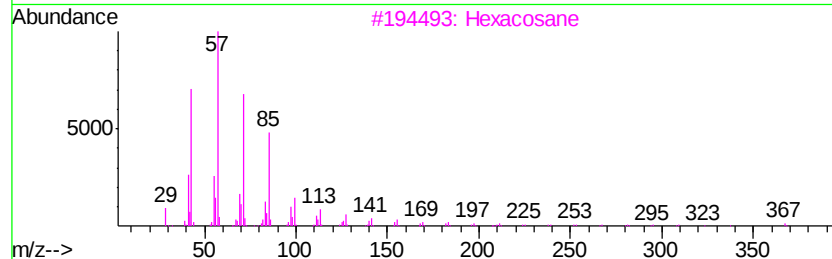
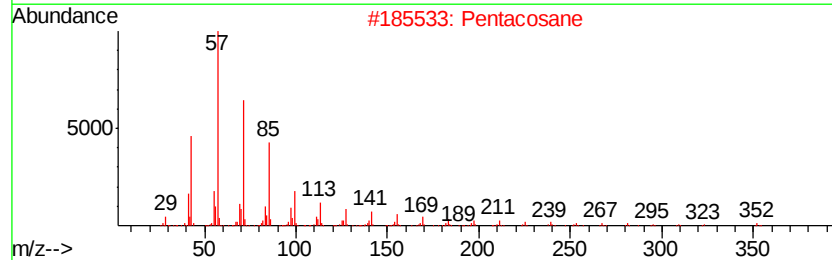
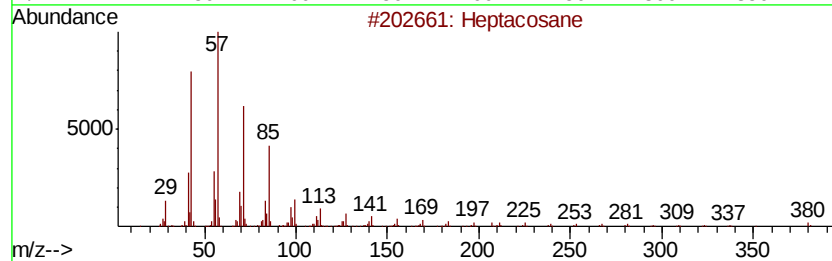
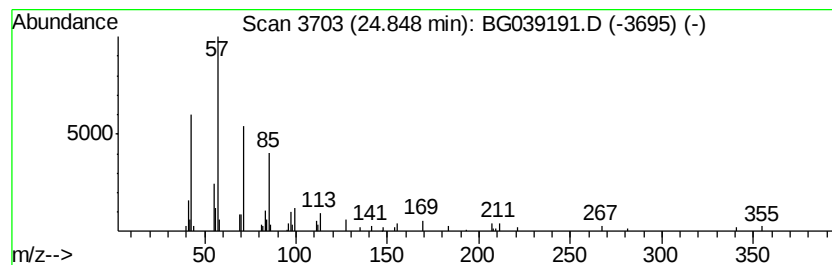
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.85	3.36 ng	76270	Perylene-d12	24.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	87
2	Pentacosane	352	C25H52	000629-99-2	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Octacosane	394	C28H58	000630-02-4	86
5	Hentriacontane	437	C31H64	000630-04-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011719\
Data File : BG039191.D
Acq On : 17 Jan 2019 18:01
Operator : JU/SJ
Sample : K1139-21
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
T-CONTAINMENT

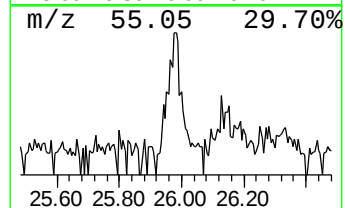
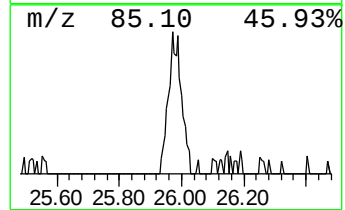
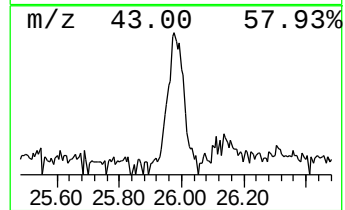
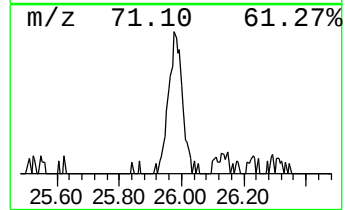
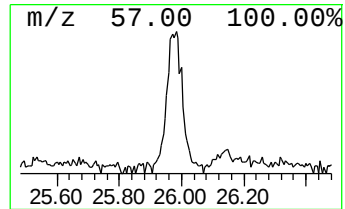
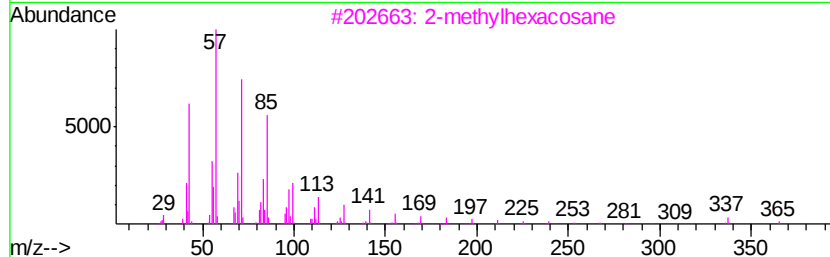
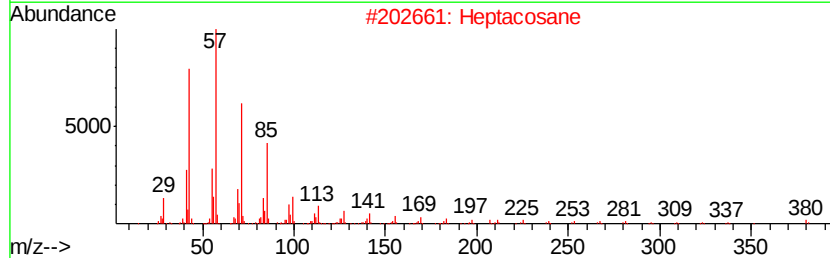
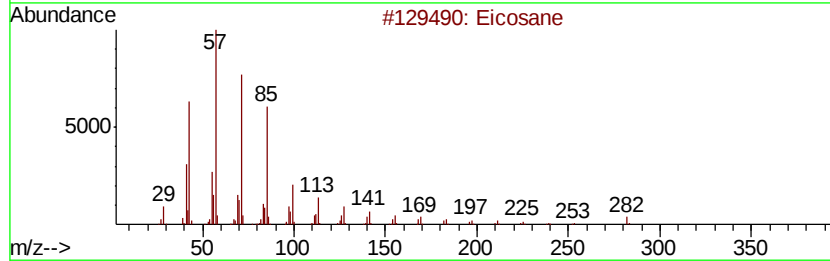
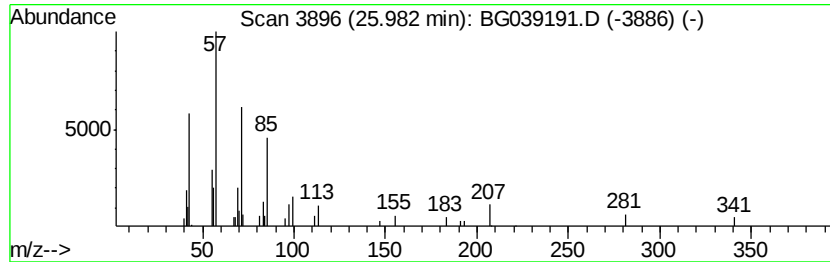
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.98	2.37 ng	53782	Perylene-d12	24.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	95
2			Heptacosane	380	C27H56	000593-49-7	83
3			2-methylhexacosane	380	C27H56	1000376-72-7	83
4			Hentriacontane	437	C31H64	000630-04-6	83
5			2-methyltetracosane	352	C25H52	1000376-72-6	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG011719\
Data File : BG039191.D
Acq On : 17 Jan 2019 18:01
Operator : JU/SJ
Sample : K1139-21
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
T-CONTAINMENT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.13	6.2	ng	37377	1	8.01	120171	20.0
unknown7.54	7.54	7.9	ng	47580	1	8.01	120171	20.0
Trifluoroacetoxy ...	21.28	4.8	ng	99441	5	21.68	418568	20.0
Methoxyacetic aci...	22.42	2.5	ng	52592	5	21.68	418568	20.0
Octacosane	23.10	3.2	ng	66293	5	21.68	418568	20.0
Squalene	23.30	4.2	ng	87970	5	21.68	418568	20.0
Heptacosane	24.85	3.4	ng	76270	6	24.94	453927	20.0
Eicosane	25.98	2.4	ng	53782	6	24.94	453927	20.0