

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040319\
 Data File : BG040353.D
 Acq On : 4 Apr 2019 9:55
 Operator : JU/SJ
 Sample : K2187-02
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-TRACK-86-87

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-BG032719.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	3.193	13	18	29	rVB	51343	102264	2.68%	0.543%
2	5.138	345	349	356	rVB	38597	59406	1.56%	0.315%
3	5.602	421	428	436	rBV	334387	539548	14.15%	2.863%
4	7.200	692	700	713	rBV	192775	350498	9.19%	1.860%
5	7.576	756	764	774	rBV	598345	1045686	27.43%	5.550%
6	8.046	837	844	857	rVB	221849	377439	9.90%	2.003%
7	8.369	891	899	907	rBV	834521	1463719	38.40%	7.768%
8	9.221	1036	1044	1061	rBV	669417	1236888	32.45%	6.564%
9	10.861	1315	1323	1331	rBV	269589	499796	13.11%	2.652%
10	13.299	1728	1738	1749	rBV	1755773	2756544	72.31%	14.629%
11	14.674	1964	1972	1979	rBV2	412858	712353	18.69%	3.781%
12	15.720	2144	2150	2157	rBV5	25901	41700	1.09%	0.221%
13	16.166	2219	2226	2237	rBV	918233	1409521	36.97%	7.481%
14	17.423	2433	2440	2449	rBV2	593765	947561	24.86%	5.029%
15	17.870	2512	2516	2523	rVB4	28120	40121	1.05%	0.213%
16	17.999	2533	2538	2543	rBV5	45483	67734	1.78%	0.359%
17	18.164	2560	2566	2574	rBV3	86530	171327	4.49%	0.909%
18	18.275	2581	2585	2593	rVB6	34282	53378	1.40%	0.283%
19	18.716	2656	2660	2667	rVB	78854	110443	2.90%	0.586%
20	20.020	2876	2882	2895	rBV	2834297	3812259	100.00%	20.232%
21	20.790	3009	3013	3017	rVB6	32699	41711	1.09%	0.221%
22	21.301	3095	3100	3109	rVB7	30947	61740	1.62%	0.328%
23	21.695	3160	3167	3177	rVB2	672137	1149769	30.16%	6.102%
24	22.441	3289	3294	3301	rVB2	44591	73194	1.92%	0.388%
25	23.134	3407	3412	3422	rVB2	59931	122990	3.23%	0.653%
26	23.945	3544	3550	3561	rVB2	70313	162843	4.27%	0.864%
27	24.897	3706	3712	3716	rBV2	58144	138227	3.63%	0.734%
28	24.968	3716	3724	3736	rVB2	394716	1145274	30.04%	6.078%
29	26.031	3898	3905	3915	rVB4	49341	148650	3.90%	0.789%

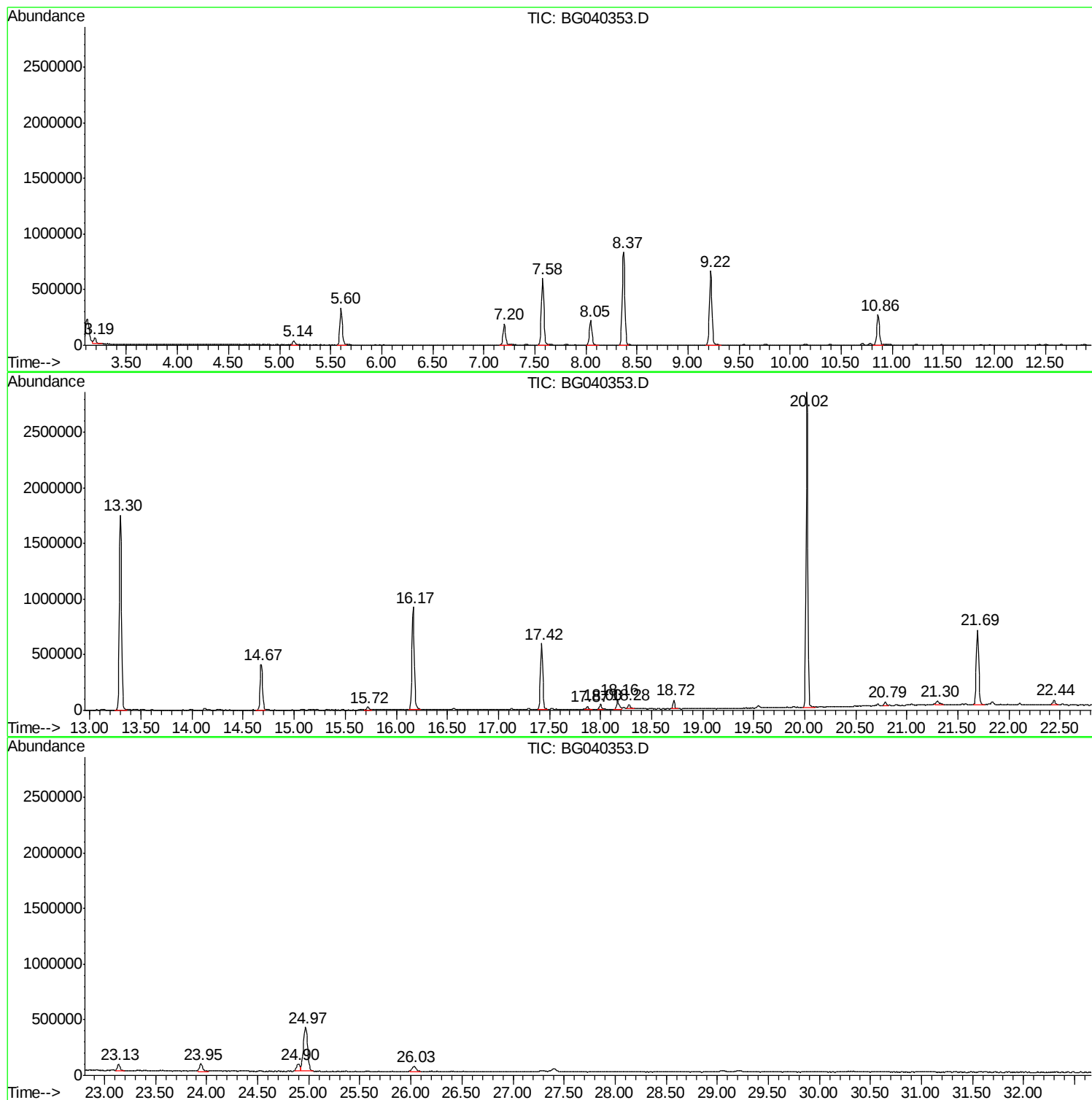
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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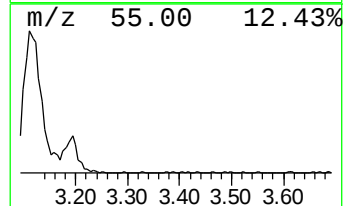
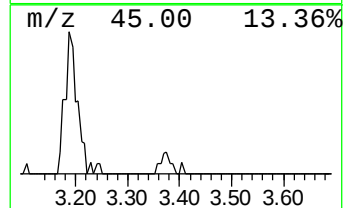
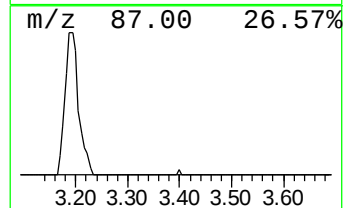
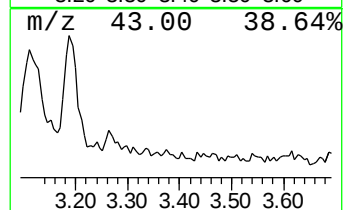
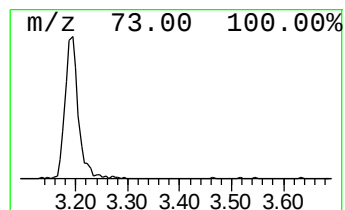
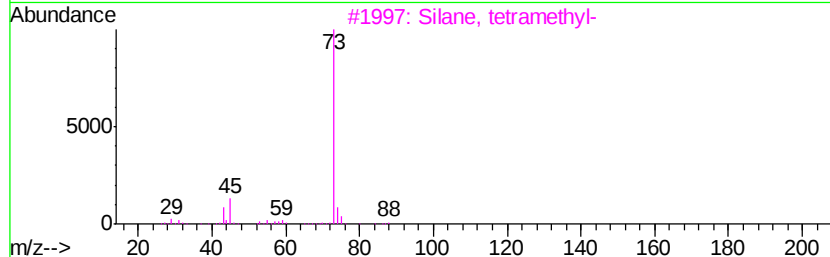
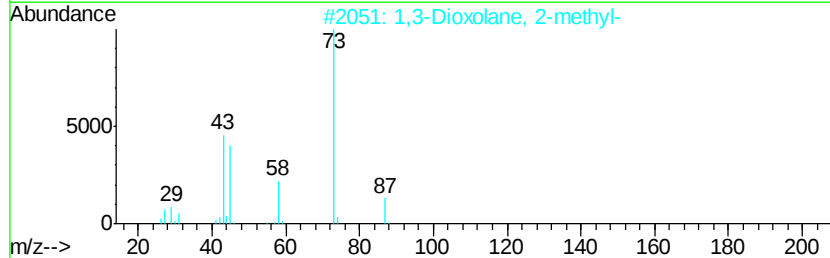
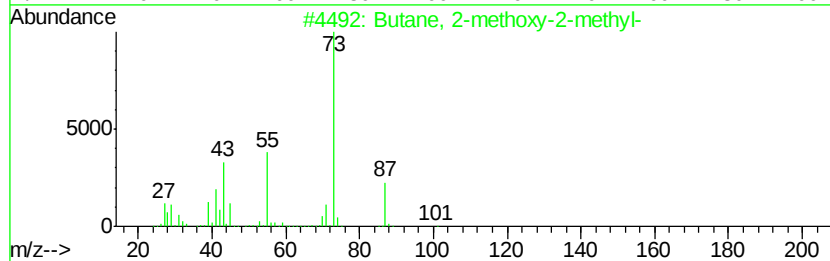
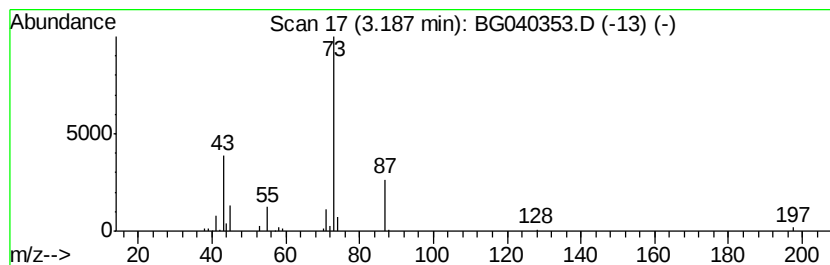
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.19	5.42 ng	102264	1,4-Dichlorobenzene-d4	8.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9



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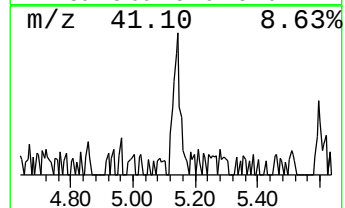
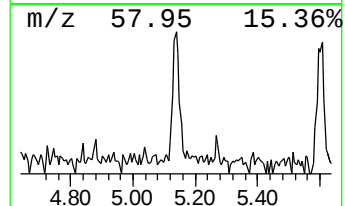
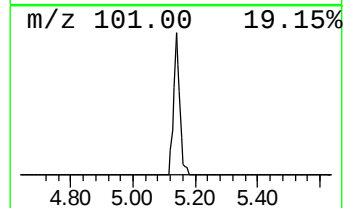
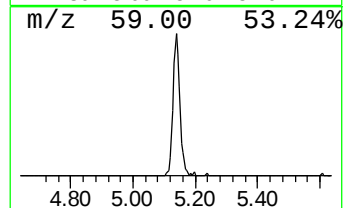
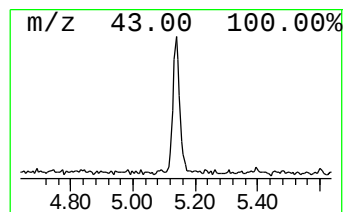
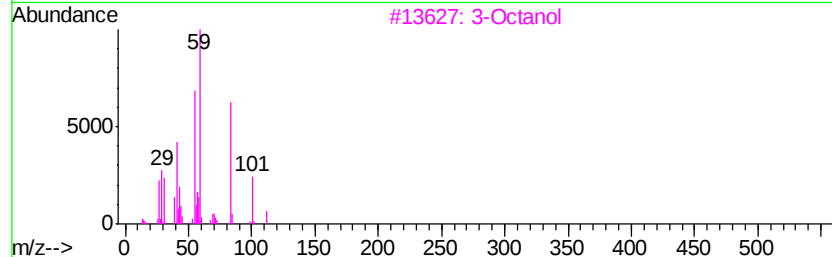
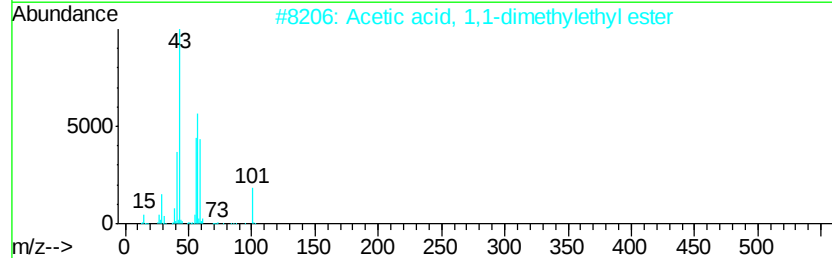
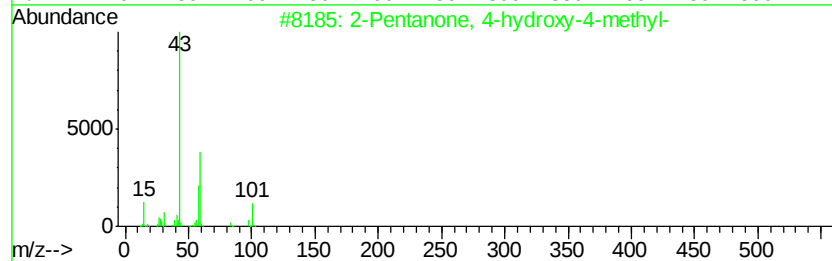
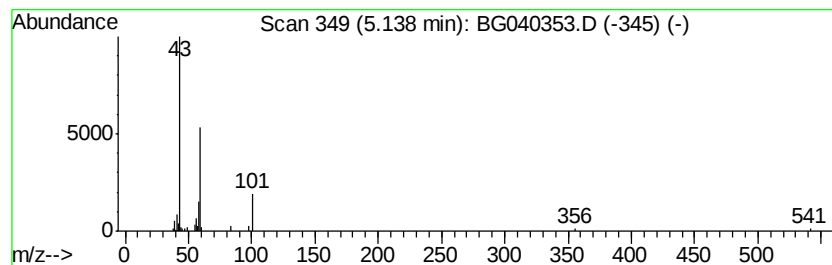
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	3.15 ng	59406	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Octanol	130	C8H18O	000589-98-0	36
4		Propanoic acid, 2-hydroxy-2-meth...	132	C6H12O3	000080-55-7	23
5		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	17



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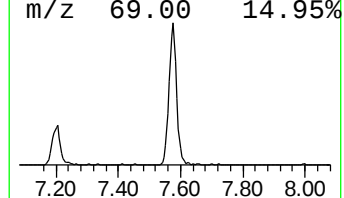
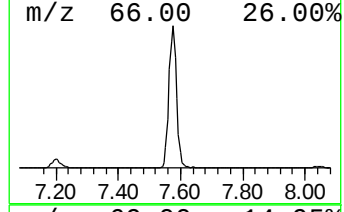
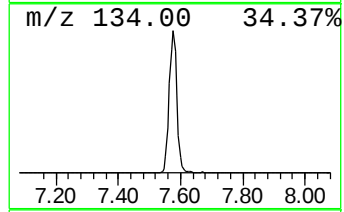
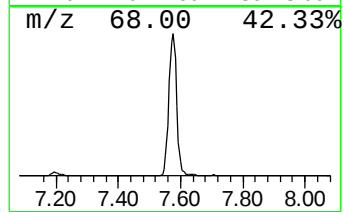
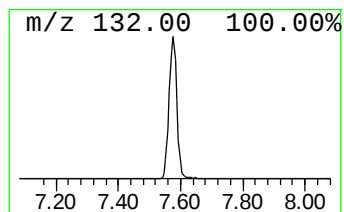
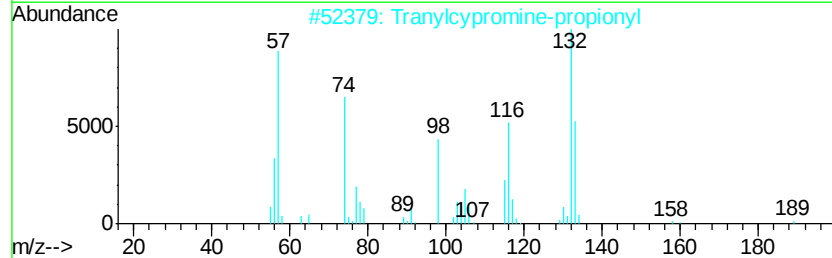
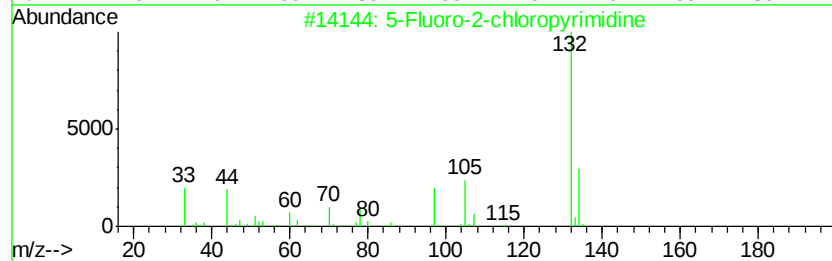
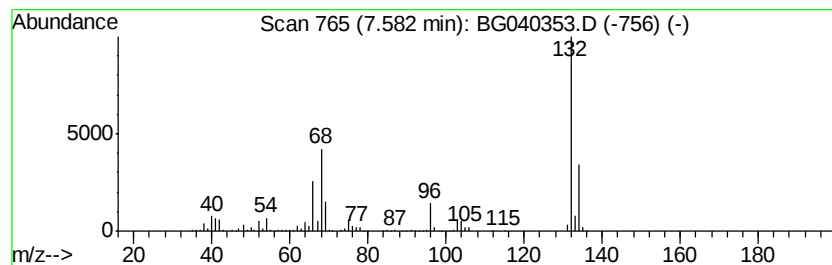
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Peak Number 3 unknown7.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	55.41 ng	1045690	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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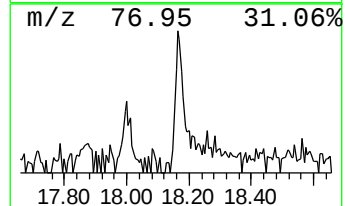
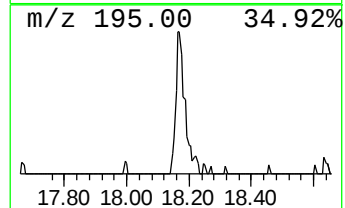
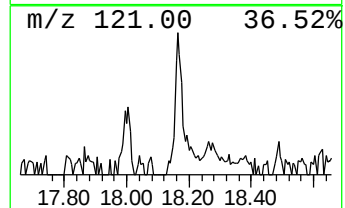
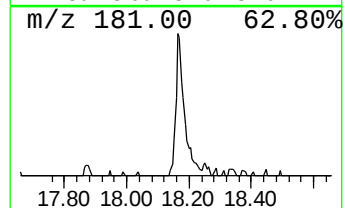
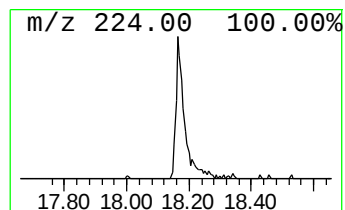
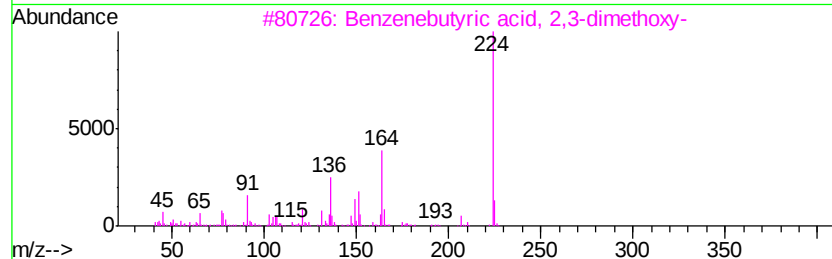
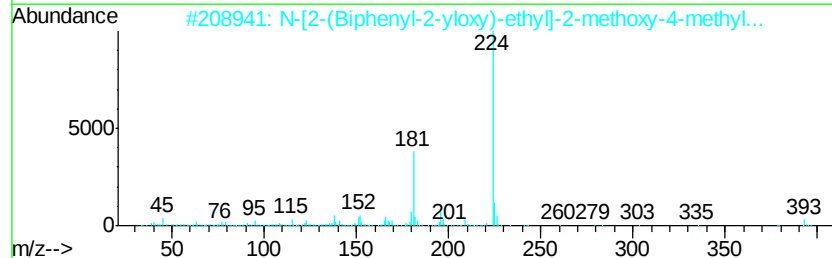
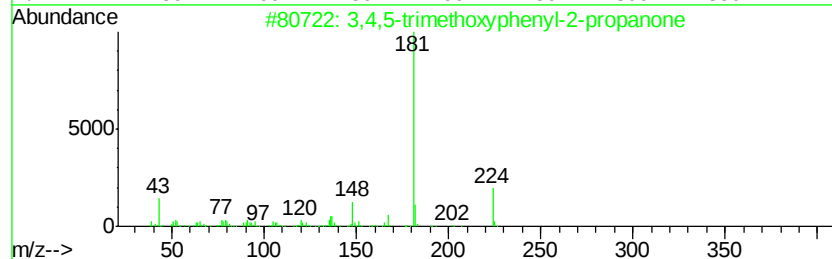
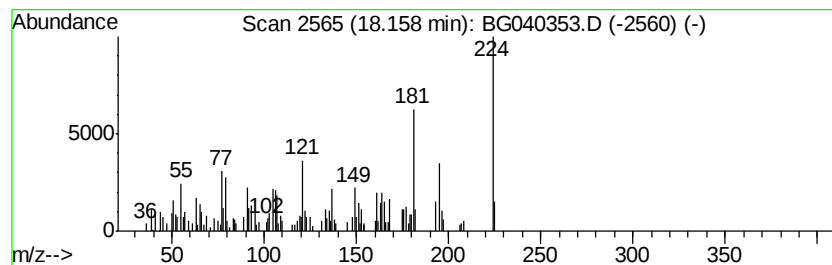
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Peak Number 5 unknown18.16 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.16	3.62 ng	171327	Phenanthrene-d10	17.42

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4,5-trimethoxyphenyl-2-propanone	224	C12H16O4	1000378-97-6	49		
2	N-[2-(Biphenyl-2-yloxy)-ethyl]-2...	393	C23H23NO3S	1000301-34-7	43		
3	Benzenebutyric acid, 2,3-dimethoxy-	224	C12H16O4	064400-76-6	41		
4	[1,2,4]Oxadiazole-5-carboxylic a...	224	C9H8N2O3S	1000316-65-0	38		
5	2-Nitro-5-thiocyanatobenzoic acid	224	C8H4N2O4S	030211-77-9	38		



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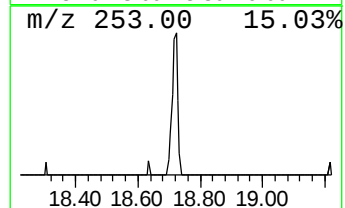
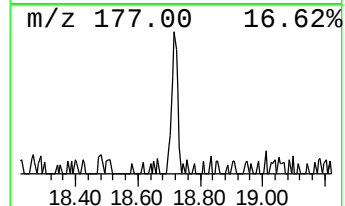
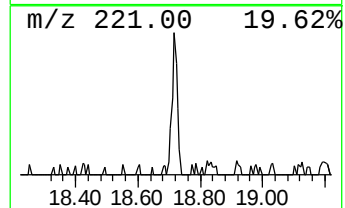
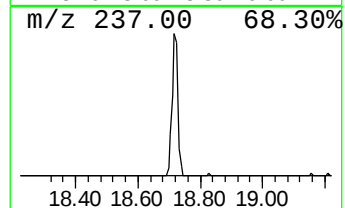
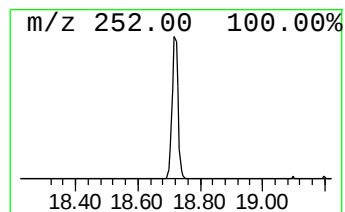
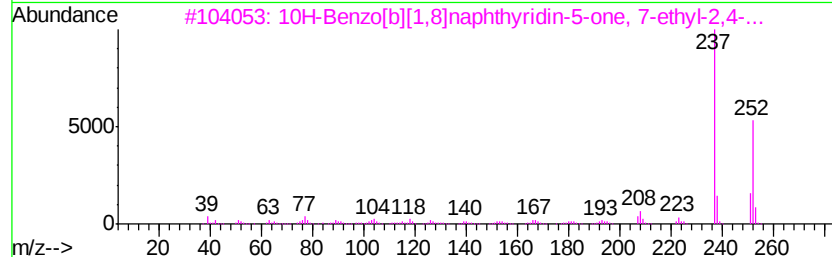
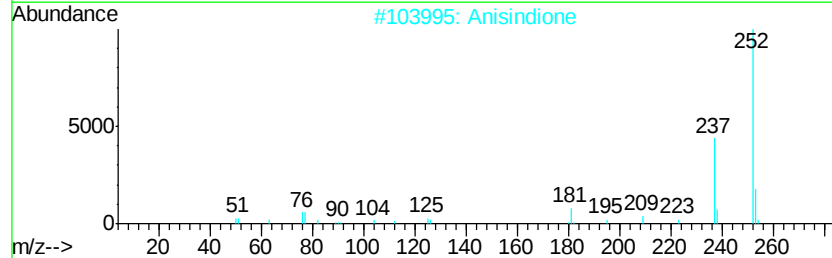
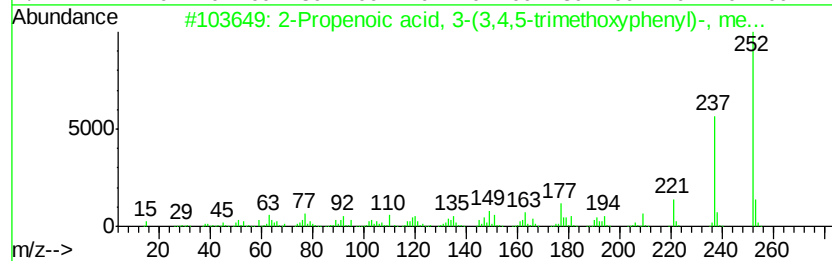
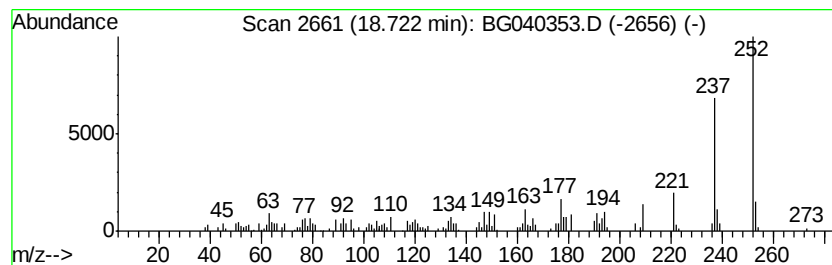
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Peak Number 6 2-Propenoic acid, 3-(3,4,5-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.72	2.33 ng	110443	Phenanthrene-d10	17.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propenoic acid, 3-(3,4,5-trime...	252	C13H16O5	007560-49-8	98
2		Anisindione	252	C16H12O3	000117-37-3	64
3		10H-Benzo[b][1,8]naphthyridin-5-...	252	C16H16N2O	1000302-05-2	59
4		3H-Pyrrolo[3,2-f]quinoline, 1,2,...	252	C17H20N2	1000338-03-5	59
5		3,4-Dihydrocoumarin, 4,4,5,7,8-p...	252	C14H17ClO2	040614-37-7	59



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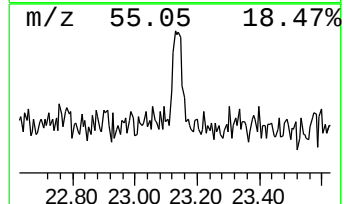
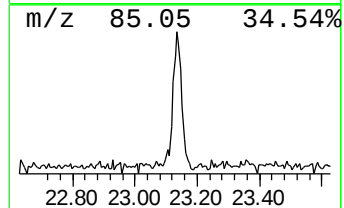
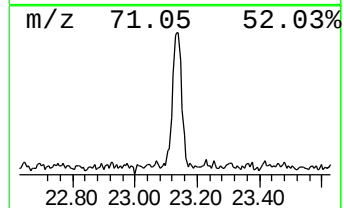
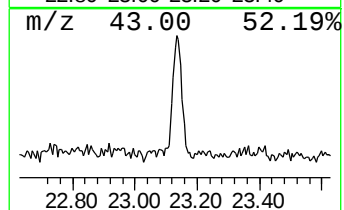
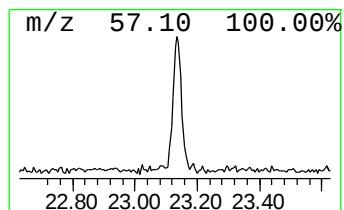
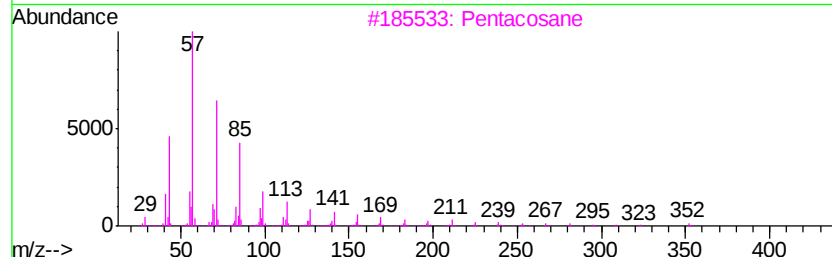
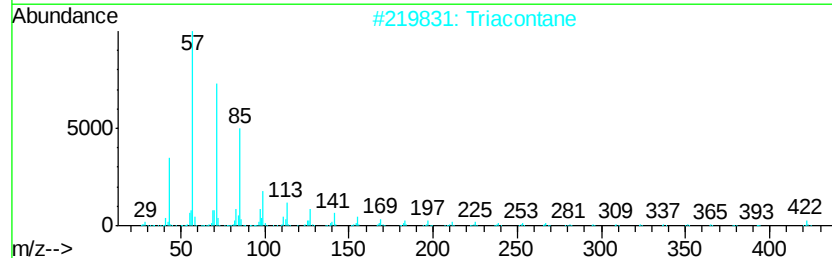
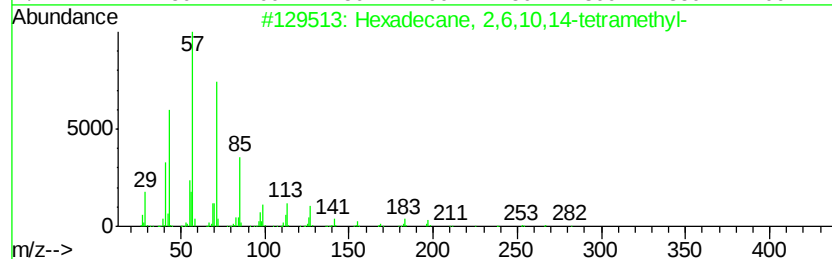
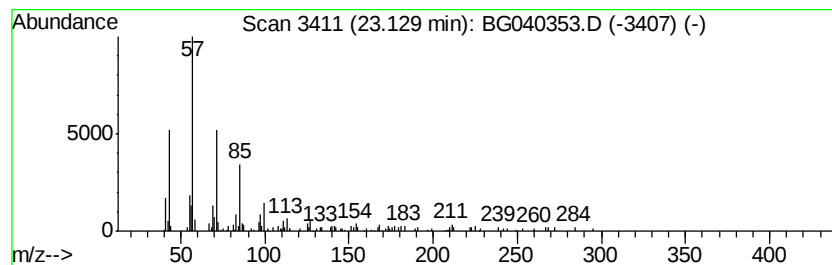
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane, 2,6,10,14-tetra... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.13	2.14 ng	122990	Chrysene-d12	21.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	93
2		Triacontane	422	C30H62	000638-68-6	91
3		Pentacosane	352	C25H52	000629-99-2	91
4		Eicosane, 2-methyl-	296	C21H44	001560-84-5	90
5		Tetracosane	338	C24H50	000646-31-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040319\
Data File : BG040353.D
Acq On : 4 Apr 2019 9:55
Operator : JU/SJ
Sample : K2187-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-TRACK-86-87

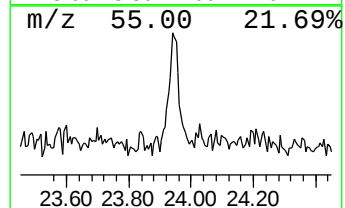
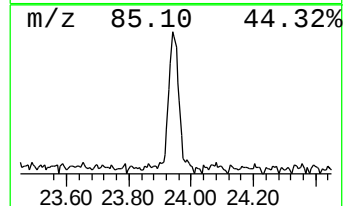
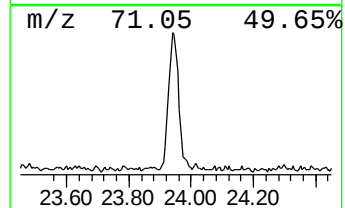
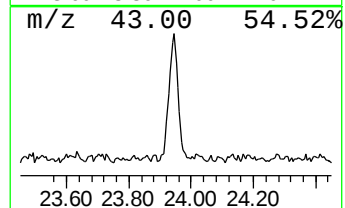
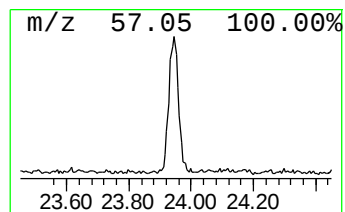
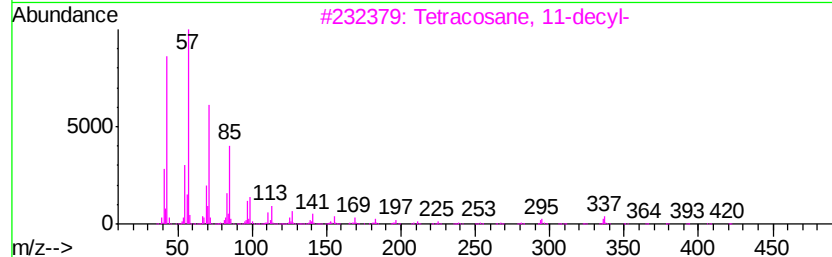
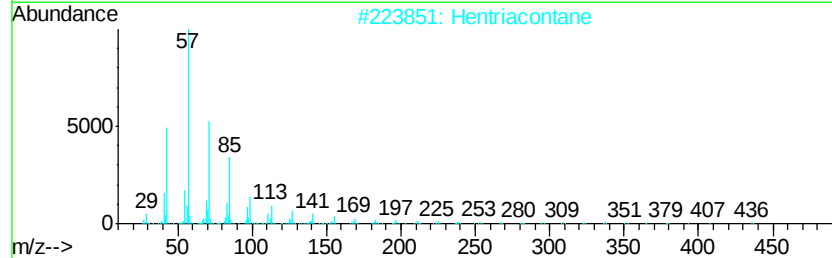
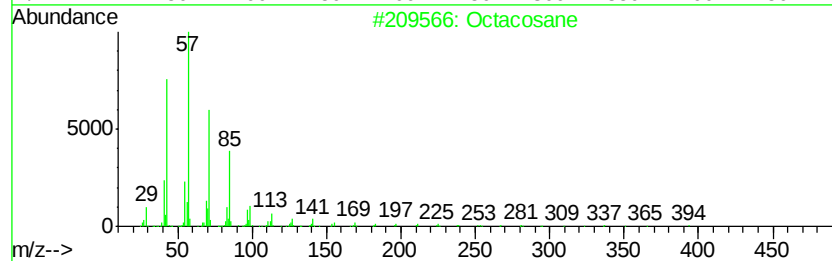
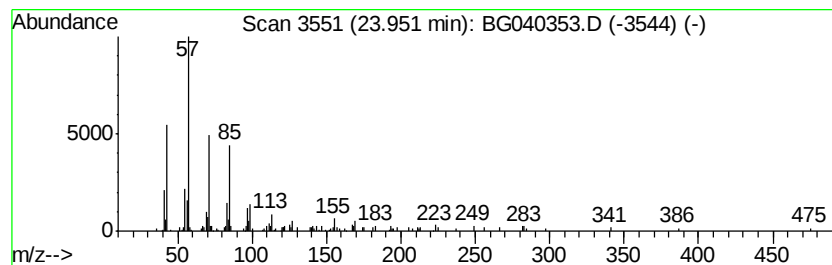
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.95	2.84 ng	162843	Perylene-d12	24.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	83
2		Hentriacontane	437	C31H64	000630-04-6	83
3		Tetracosane, 11-decyl-	479	C34H70	055429-84-0	80
4		Tetracosane	338	C24H50	000646-31-1	80
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040319\
Data File : BG040353.D
Acq On : 4 Apr 2019 9:55
Operator : JU/SJ
Sample : K2187-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-TRACK-86-87

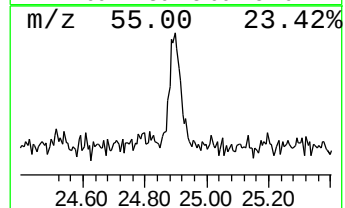
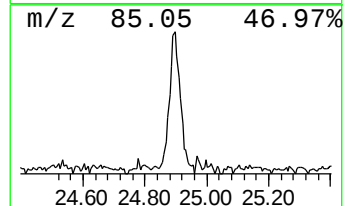
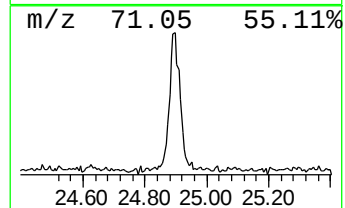
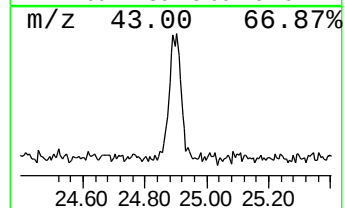
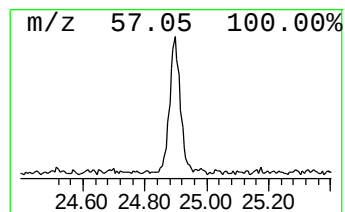
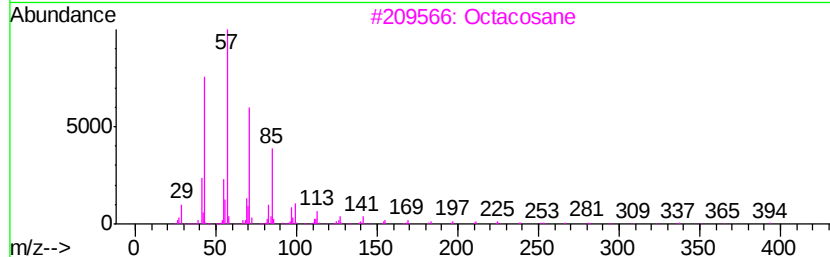
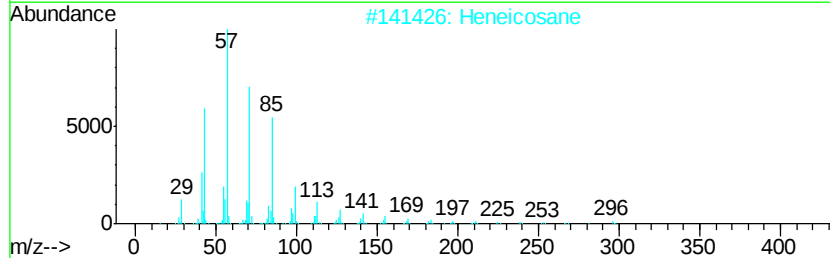
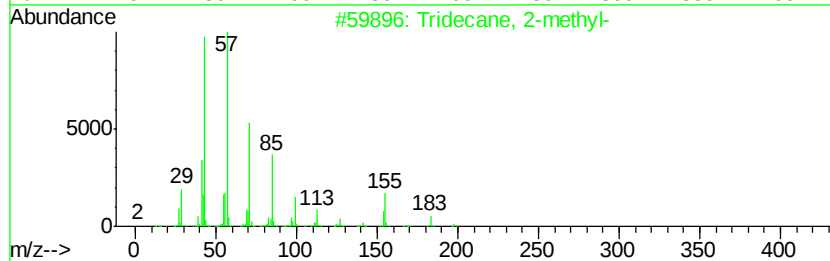
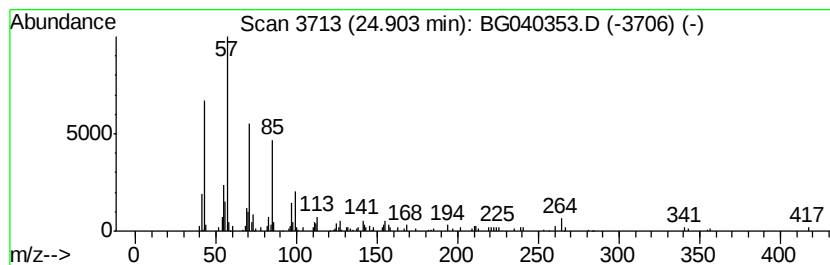
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tridecane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.90	2.41 ng	138227	Perylene-d12	24.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane, 2-methyl-	198	C14H30	001560-96-9	87
2		Heneicosane	296	C21H44	000629-94-7	86
3		Octacosane	394	C28H58	000630-02-4	86
4		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86
5		Docosane	310	C22H46	000629-97-0	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040319\
Data File : BG040353.D
Acq On : 4 Apr 2019 9:55
Operator : JU/SJ
Sample : K2187-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-TRACK-86-87

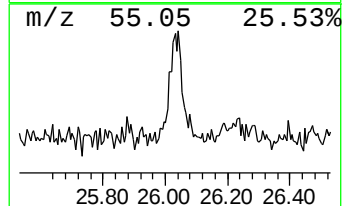
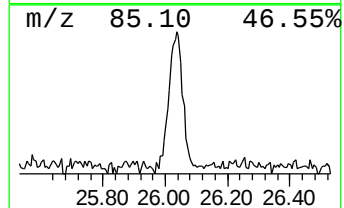
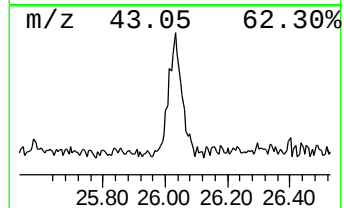
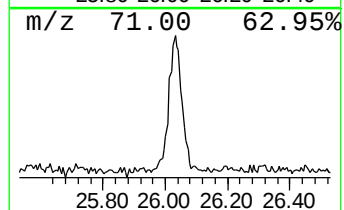
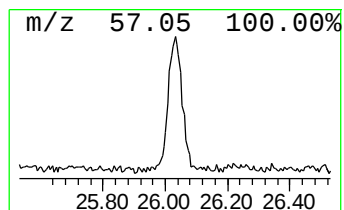
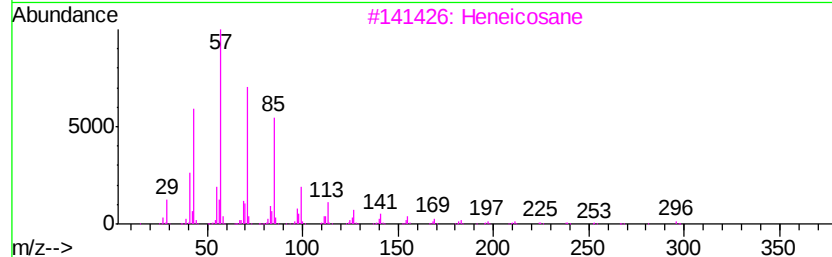
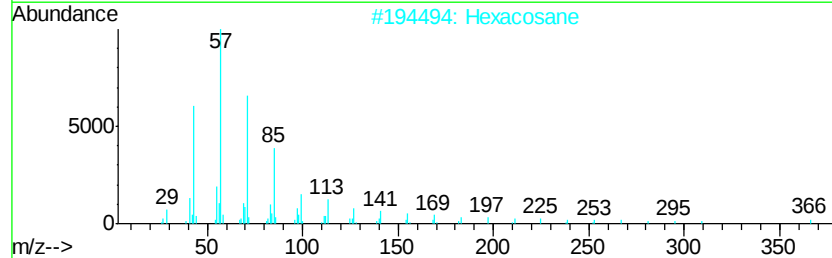
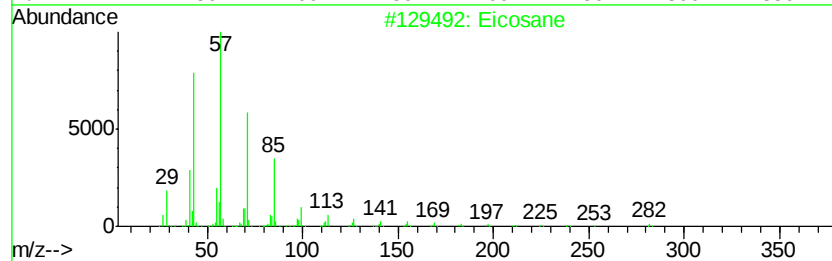
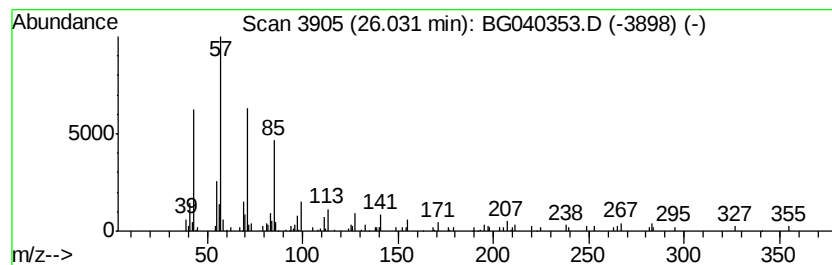
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.03	2.60 ng	148650	Perylene-d12	24.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	93
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heneicosane	296	C21H44	000629-94-7	87
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5		Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040319\
Data File : BG040353.D
Acq On : 4 Apr 2019 9:55
Operator : JU/SJ
Sample : K2187-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-TRACK-86-87

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.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...	3.19	5.4	ng	102264	1	8.05	377439	20.0
2-Pentanone, 4-hy...	5.14	3.1	ng	59406	1	8.05	377439	20.0
unknown7.58	7.58	55.4	ng	1045690	1	8.05	377439	20.0
unknown18.16	18.16	3.6	ng	171327	4	17.42	947561	20.0
2-Propenoic acid,...	18.72	2.3	ng	110443	4	17.42	947561	20.0
Hexadecane, 2,6,1...	23.13	2.1	ng	122990	5	21.69	1149770	20.0
Octacosane	23.95	2.8	ng	162843	6	24.97	1145270	20.0
Tridecane, 2-methyl-	24.90	2.4	ng	138227	6	24.97	1145270	20.0
Eicosane	26.03	2.6	ng	148650	6	24.97	1145270	20.0