

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG090820\
 Data File : BG046566.D
 Acq On : 8 Sep 2020 20:37
 Operator : CG/JU
 Sample : L3919-17
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-15

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-BG082520.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	3.124	3	6	22	rVB	285834	423504	11.58%	2.124%
2	5.515	406	413	423	rBV	744781	1184219	32.39%	5.938%
3	7.101	672	683	702	rBV	743455	1315128	35.97%	6.595%
4	7.930	817	824	832	rBV	233137	401438	10.98%	2.013%
5	9.081	1012	1020	1033	rBV	486859	897391	24.55%	4.500%
6	10.726	1291	1300	1309	rBV	331673	602810	16.49%	3.023%
7	13.182	1711	1718	1734	rBV	1418450	2346653	64.19%	11.767%
8	14.011	1853	1859	1871	rBV	65916	109139	2.99%	0.547%
9	14.557	1945	1952	1964	rBV	587201	926867	25.35%	4.648%
10	16.044	2198	2205	2216	rBV	1090021	1769365	48.40%	8.872%
11	17.301	2411	2419	2433	rBV	739642	1186542	32.45%	5.950%
12	18.206	2567	2573	2580	rBV	102546	184699	5.05%	0.926%
13	18.476	2615	2619	2625	rBV6	26786	37660	1.03%	0.189%
14	19.128	2725	2730	2739	rBV	87584	152409	4.17%	0.764%
15	19.357	2765	2769	2771	rBV	26574	38608	1.06%	0.194%
16	19.598	2806	2810	2818	rBV	29033	56850	1.55%	0.285%
17	19.916	2858	2864	2871	rBV	2691344	3656015	100.00%	18.333%
18	20.456	2952	2956	2964	rBV	171459	291827	7.98%	1.463%
19	21.214	3081	3085	3100	rVB	367308	593067	16.22%	2.974%
20	21.549	3136	3142	3148	rVB2	764988	1213482	33.19%	6.085%
21	22.137	3238	3242	3251	rVB	78735	145542	3.98%	0.730%
22	22.360	3277	3280	3291	rVB3	112288	249049	6.81%	1.249%
23	23.341	3442	3447	3454	rVB	129844	232710	6.37%	1.167%
24	23.782	3518	3522	3527	rBV2	49511	81991	2.24%	0.411%
25	23.840	3527	3532	3544	rVB	136868	324574	8.88%	1.628%
26	24.645	3661	3669	3684	rVB2	438450	1281495	35.05%	6.426%
27	25.773	3856	3861	3871	rVB2	91807	239195	6.54%	1.199%

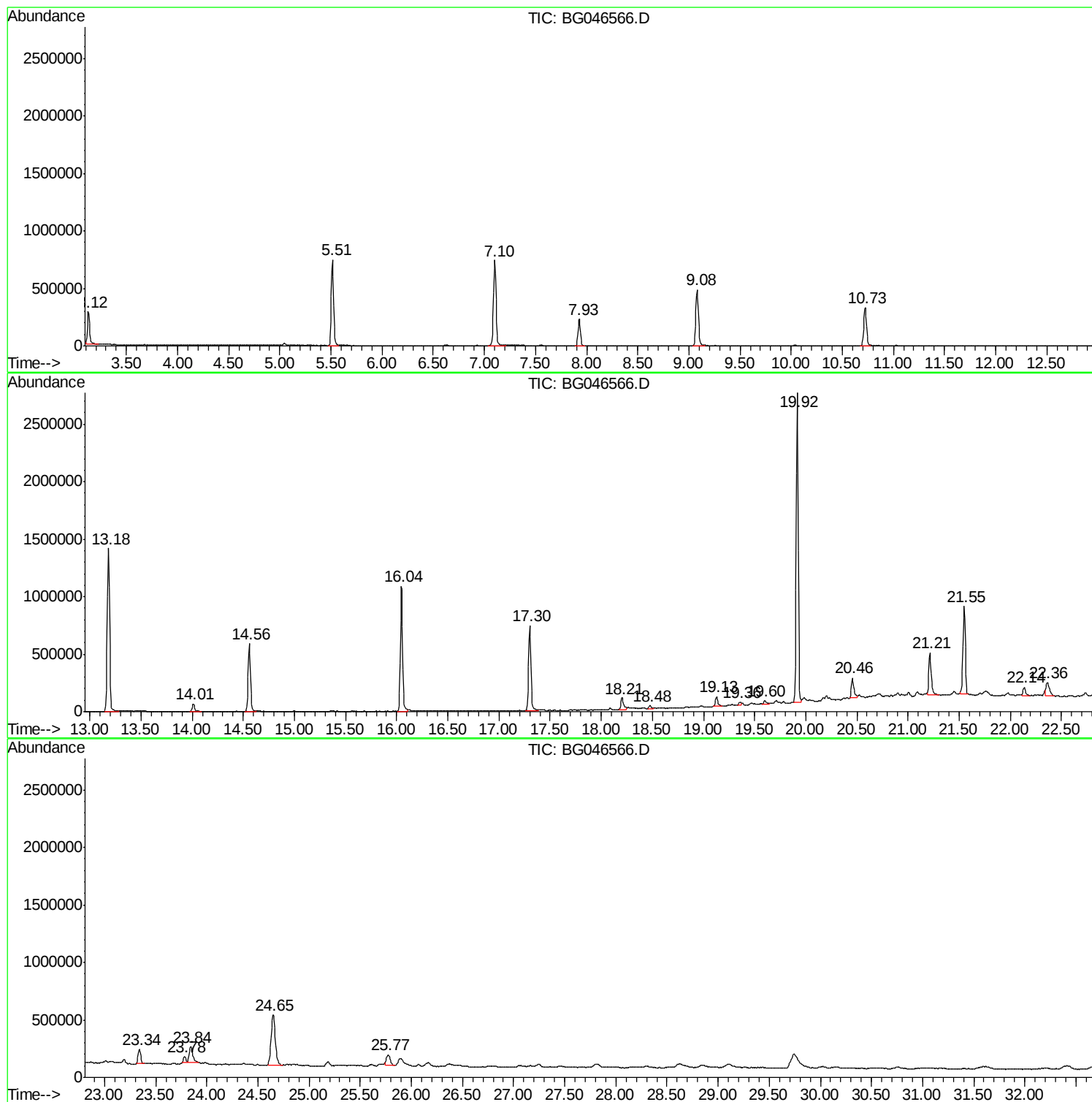
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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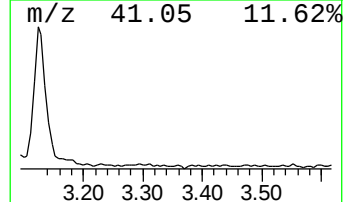
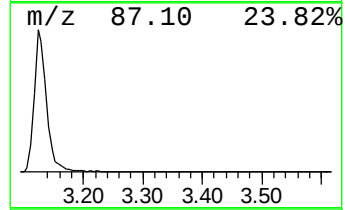
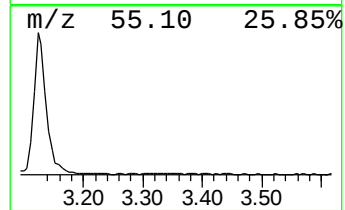
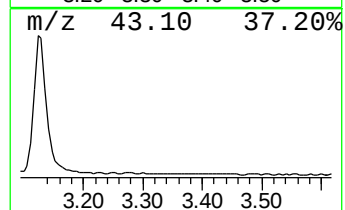
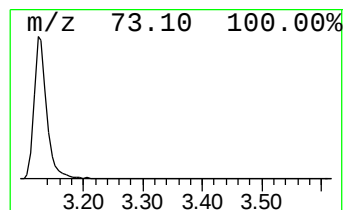
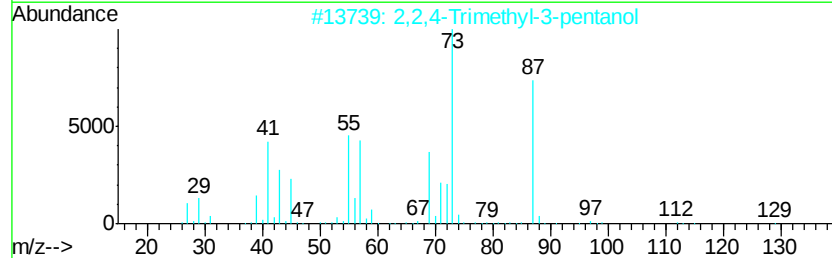
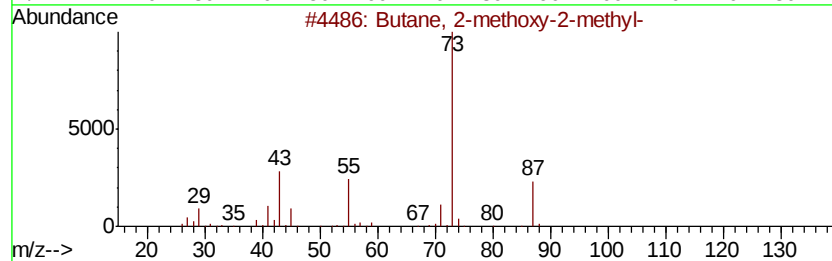
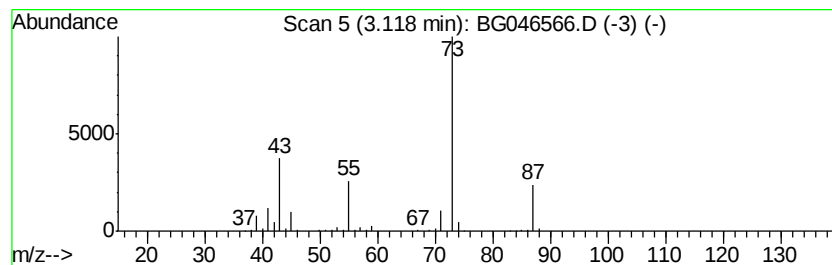
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	21.10 ng	423504	1,4-Dichlorobenzene-d4	7.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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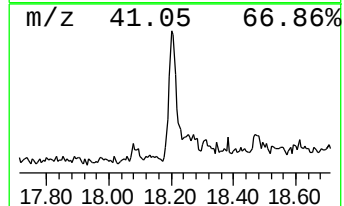
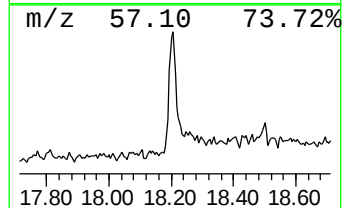
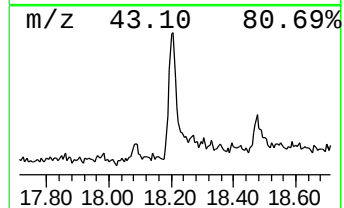
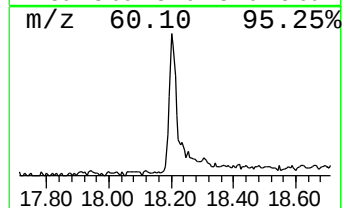
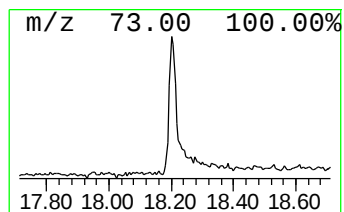
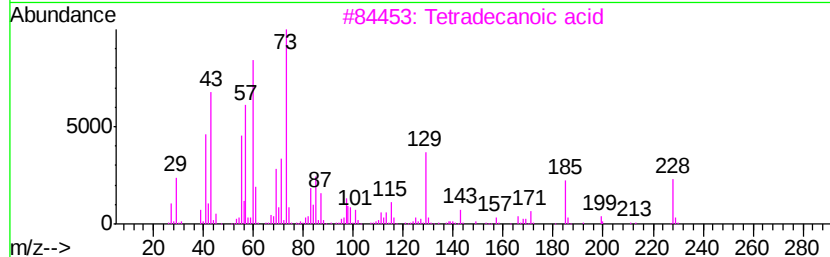
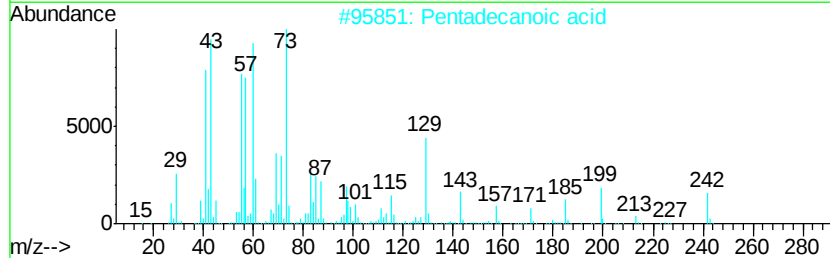
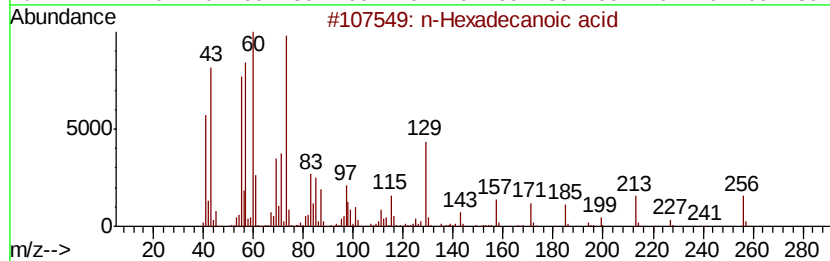
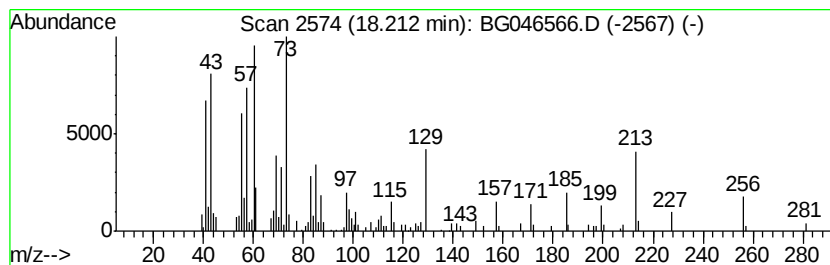
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.21	3.11 ng	184699	Phenanthrene-d10		17.30
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Undecanoic acid	186	C11H22O2	000112-37-8	68
5	Nonanoic acid	158	C9H18O2	000112-05-0	38



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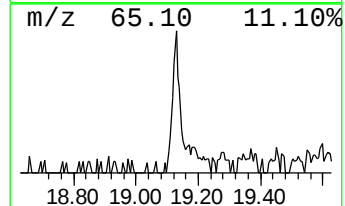
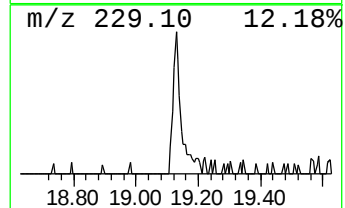
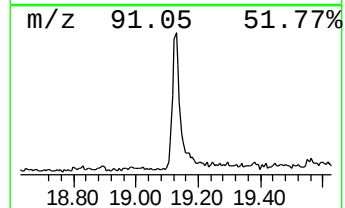
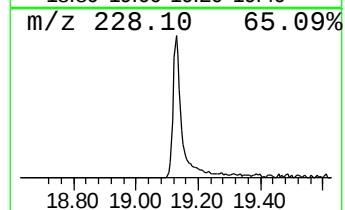
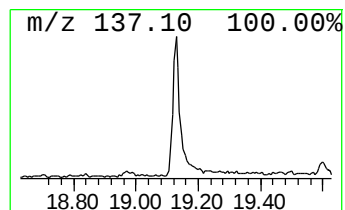
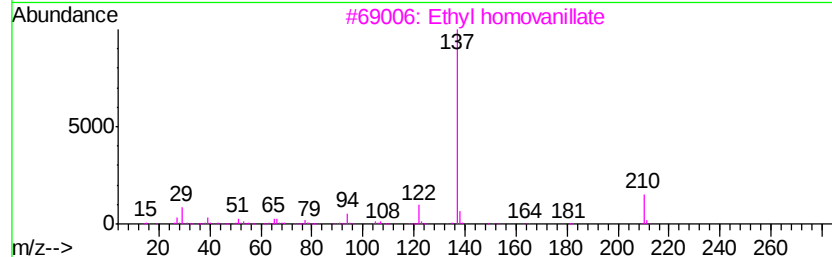
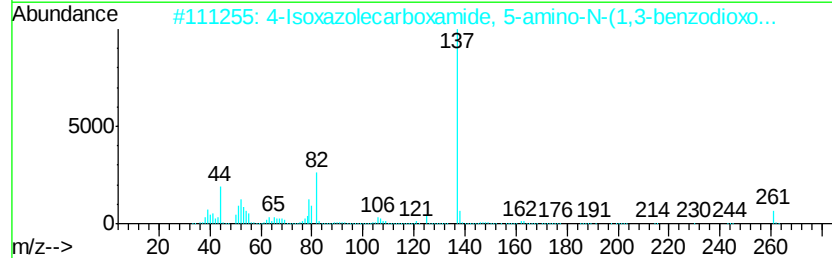
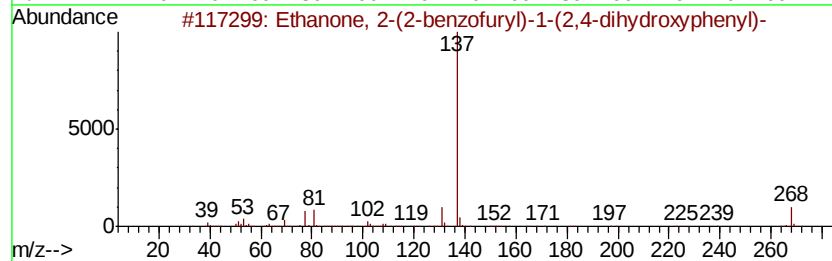
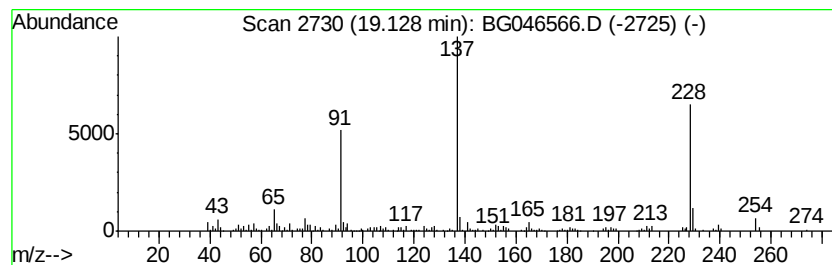
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Peak Number 3 unknown19.13 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.13	2.57 ng	152409	Phenanthrene-d10	17.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanone, 2-(2-benzofurvl)-1-(2,...	268	C16H12O4	036754-59-3	38
2		4-Isoxazolecarboxamide, 5-amino-...	261	C12H11N3O4	1000337-98-2	32
3		Ethyl homovanillate	210	C11H14O4	060563-13-5	32
4		(4-Methoxy-phenyl)-(2-nitrocyclo...	265	C14H19NO4	103077-68-5	32
5		2',4'-Dihydroxyacetophenone, dia...	236	C12H12O5	1000352-81-9	32



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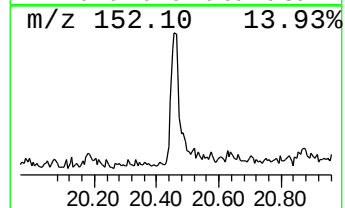
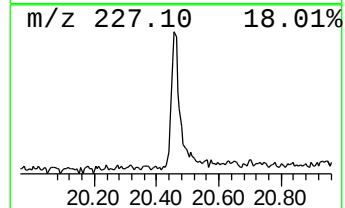
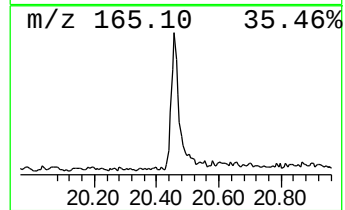
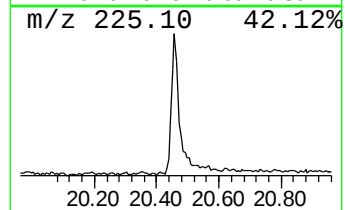
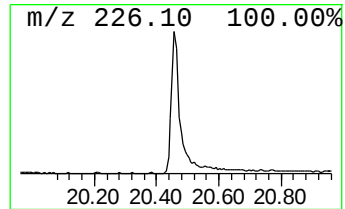
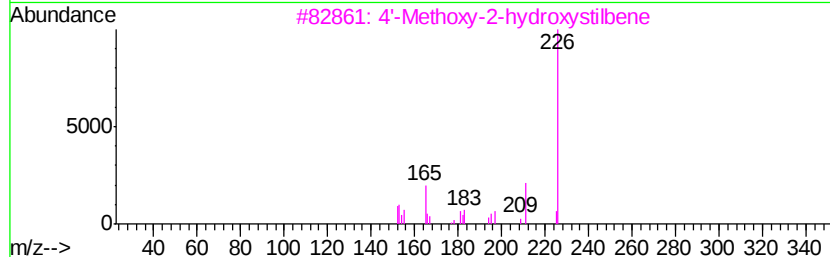
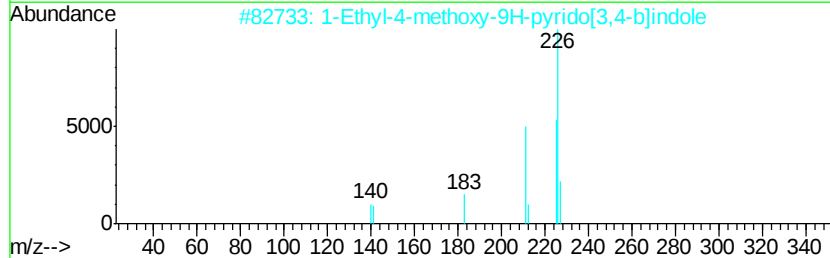
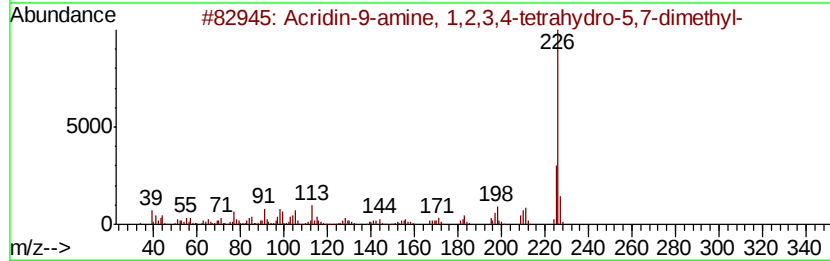
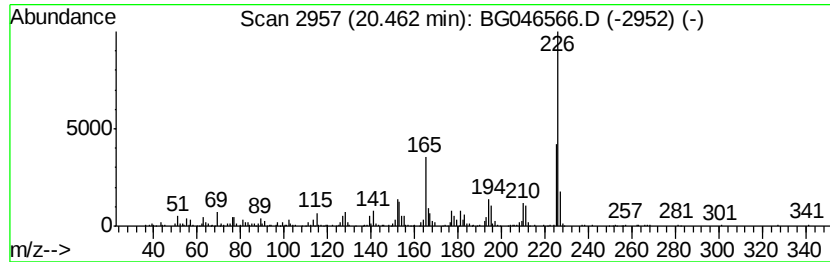
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Peak Number 4 unknown20.46 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.46	4.81 ng	291827	Chrysene-d12	21.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acridin-9-amine, 1,2,3,4-tetrahy...	226	C15H18N2	1000300-57-6	46
2		1-Ethyl-4-methoxy-9H-pyrido[3,4-...	226	C14H14N2O	026585-14-8	43
3		4'-Methoxy-2-hydroxystilbene	226	C15H14O2	1000147-93-1	43
4		9H-Xanthen-9-one, 3-methoxy-	226	C14H10O3	003722-52-9	42
5		1,3-Diamino-5,6-dihydro-7-methyl...	226	C13H14N4	037436-37-6	38



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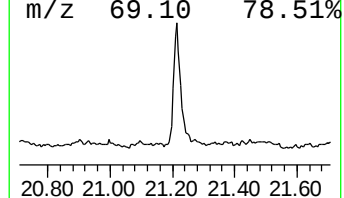
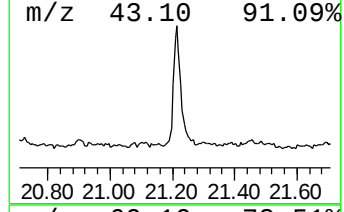
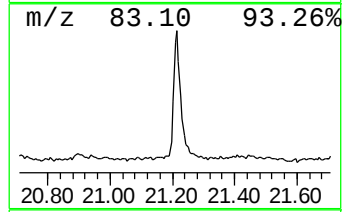
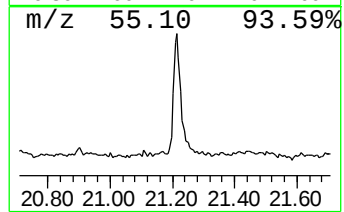
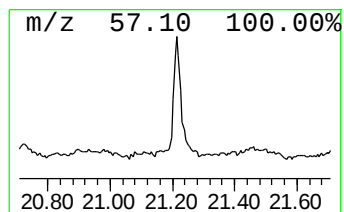
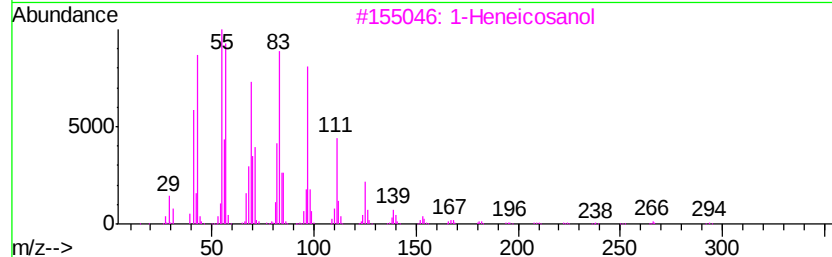
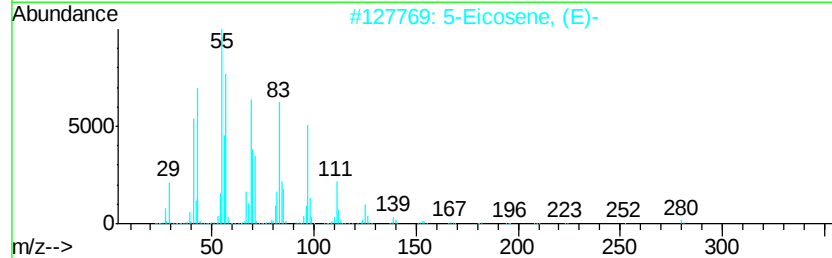
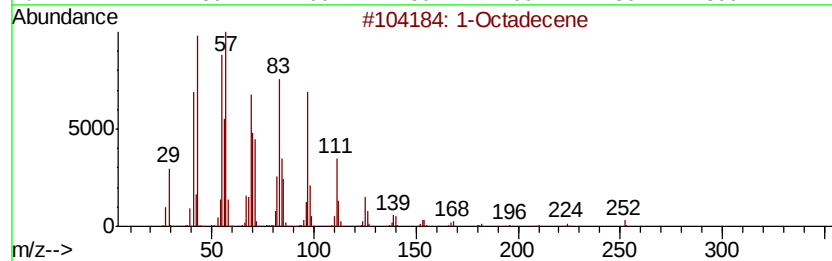
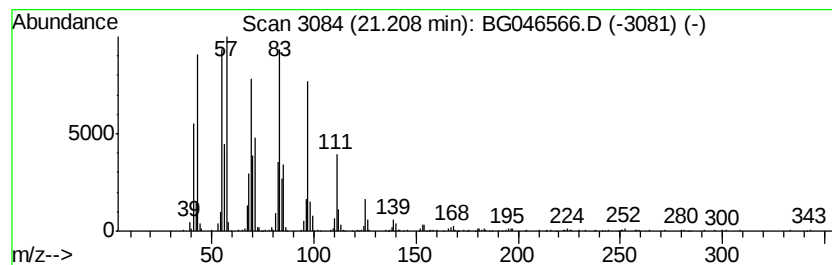
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Peak Number 5 1-Octadecene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.21	9.77 ng	593067	Chrysene-d12	21.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Octadecene	252	C18H36	000112-88-9	98
2		5-Eicosene, (E)-	280	C20H40	074685-30-6	97
3		1-Heneicosanol	312	C21H44O	015594-90-8	95
4		Behenic alcohol	326	C22H46O	000661-19-8	94
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	94



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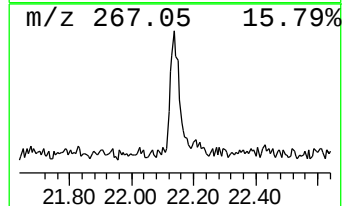
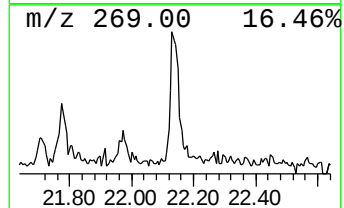
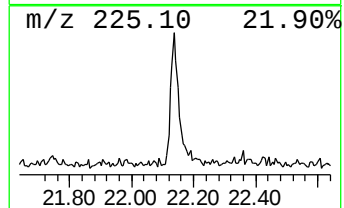
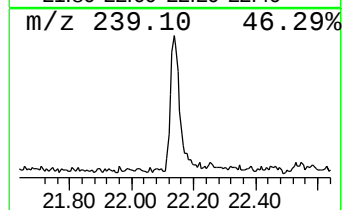
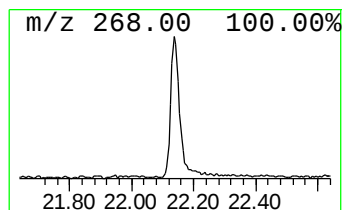
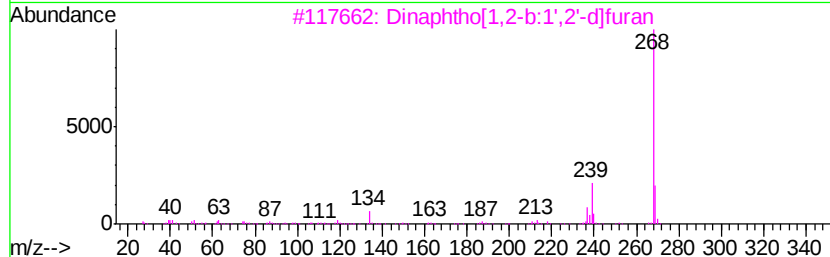
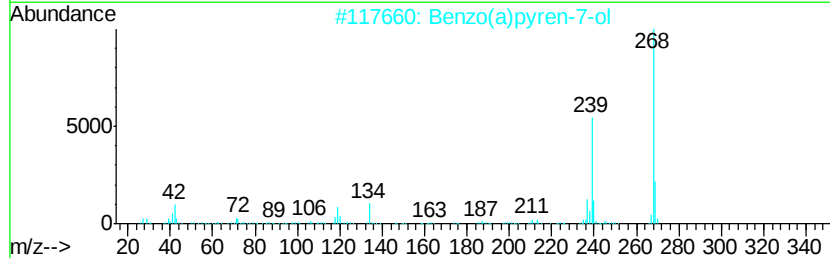
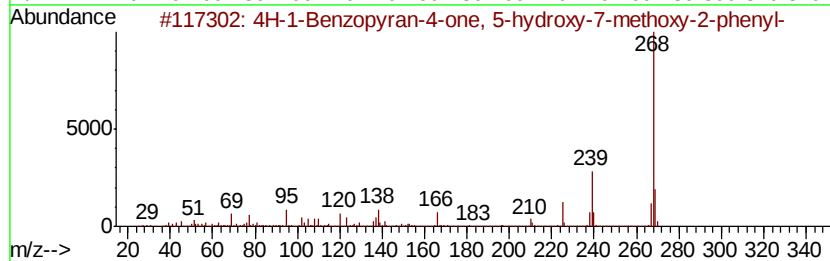
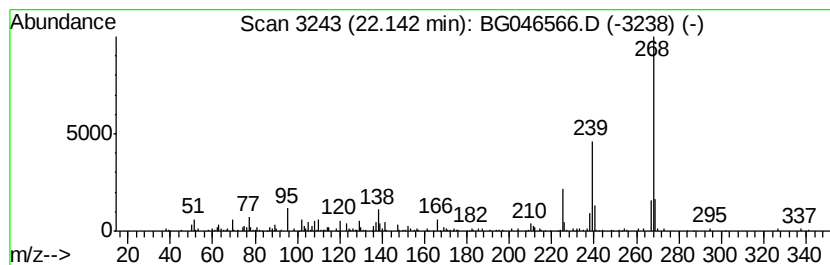
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 4H-1-Benzopyran-4-one, 5-hy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.14	2.40 ng	145542	Chrysene-d12	21.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4H-1-Benzopyran-4-one, 5-hydroxy...	268	C16H12O4	000520-28-5	76
2		Benzo(a)pyren-7-ol	268	C20H12O	037994-82-4	70
3		Dinaphtho[1,2-b:1',2'-d]furan	268	C20H12O	000207-93-2	58
4		Dinaphtho[2,1-b:1',2'-d]furan	268	C20H12O	000194-63-8	58
5		4H-1-Benzopyran-4-one, 7-hydroxy...	268	C16H12O4	000487-24-1	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG090820\
Data File : BG046566.D
Acq On : 8 Sep 2020 20:37
Operator : CG/JU
Sample : L3919-17
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-15

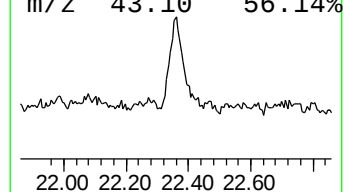
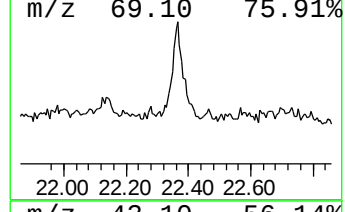
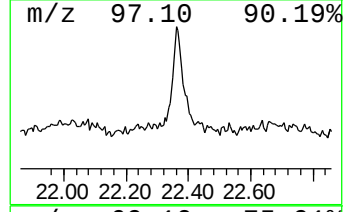
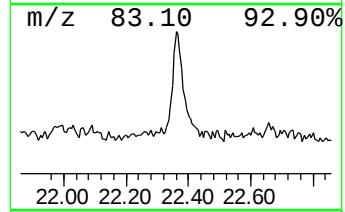
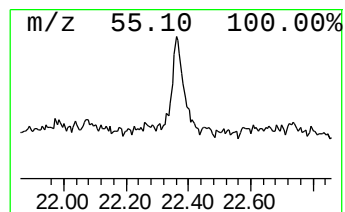
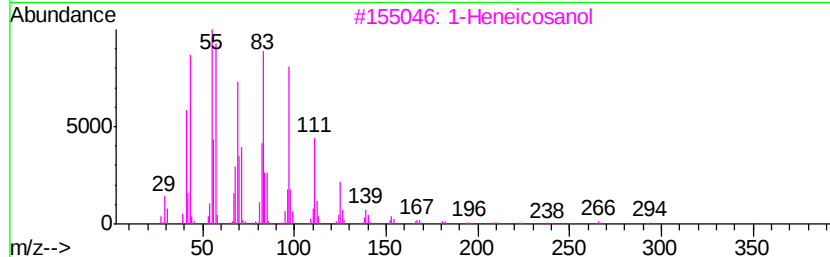
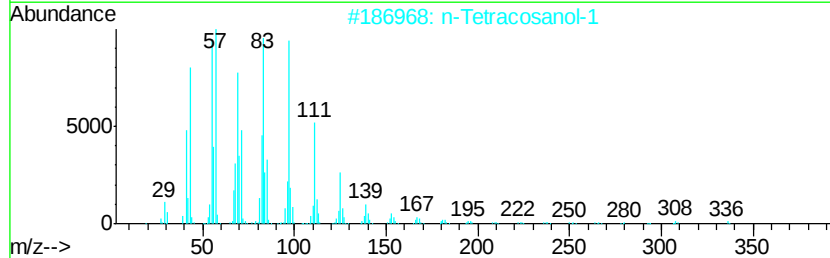
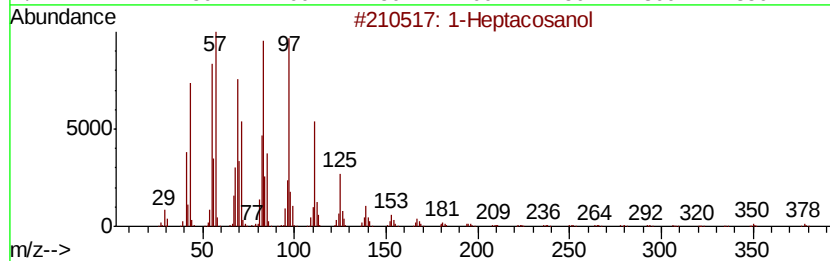
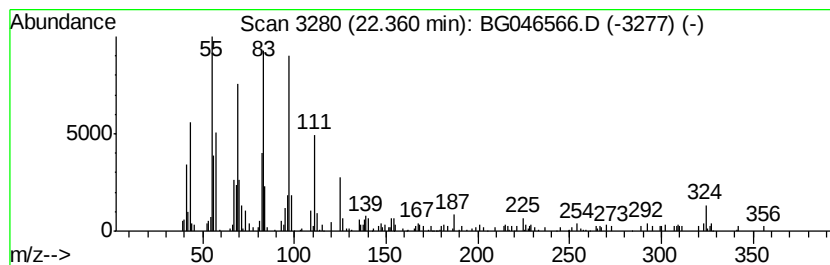
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.36	4.10 ng	249049	Chrysene-d12	21.55

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol		396	C27H56O	002004-39-9	91
2	n-Tetracosanol-1		354	C24H50O	000506-51-4	90
3	1-Heneicosanol		312	C21H44O	015594-90-8	83
4	1-Nonadecene		266	C19H38	018435-45-5	83
5	Octacosanol		410	C28H58O	000557-61-9	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG090820\
 Data File : BG046566.D
 Acq On : 8 Sep 2020 20:37
 Operator : CG/JU
 Sample : L3919-17
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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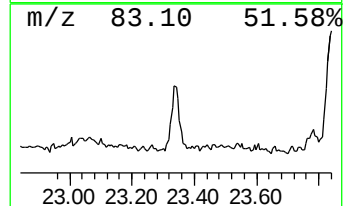
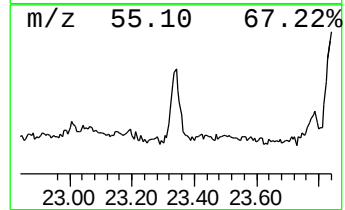
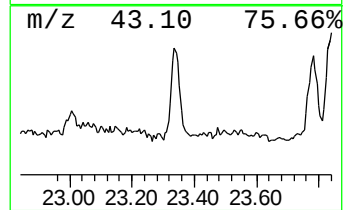
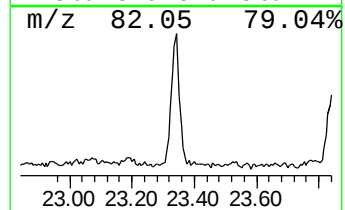
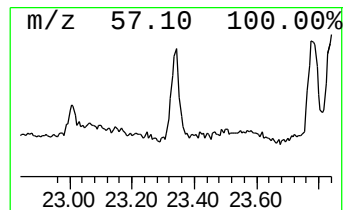
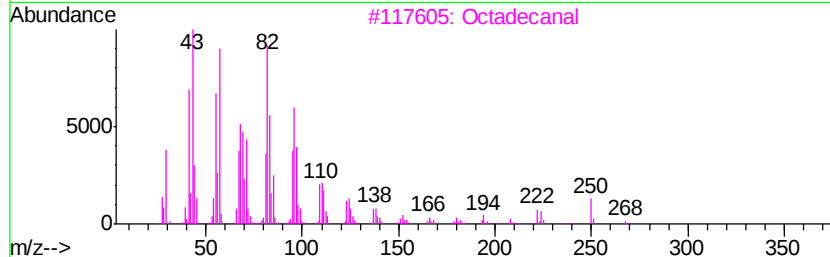
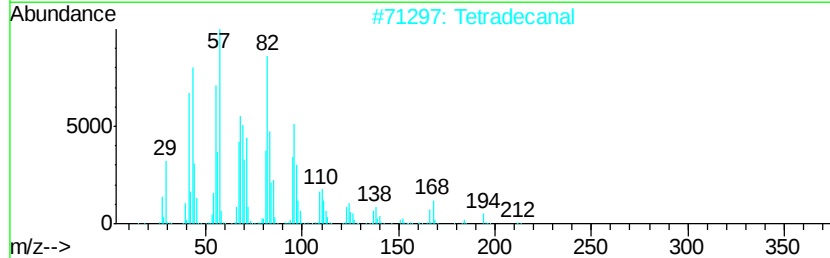
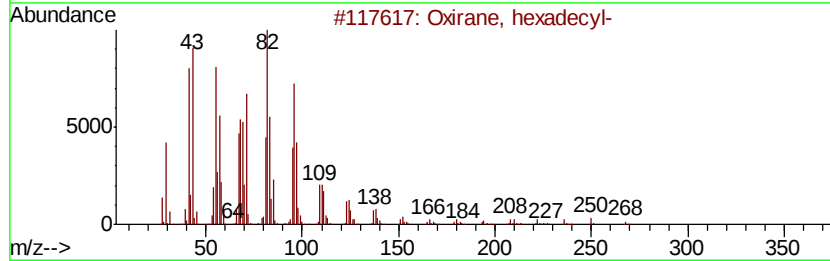
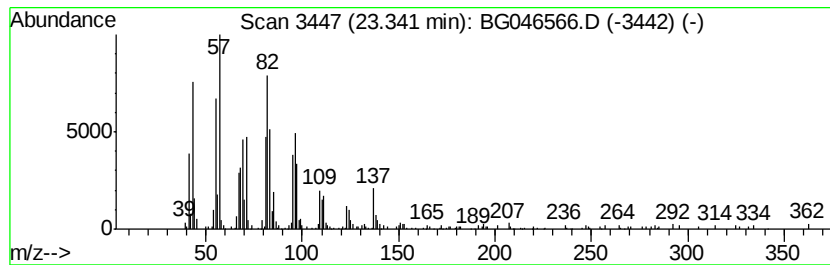
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Oxirane, hexadecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.34	3.63 ng	232710	Perylene-d12	24.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90
2		Tetradecanal	212	C14H28O	000124-25-4	87
3		Octadecanal	268	C18H36O	000638-66-4	86
4		18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	76
5		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG090820\
Data File : BG046566.D
Acq On : 8 Sep 2020 20:37
Operator : CG/JU
Sample : L3919-17
Misc :
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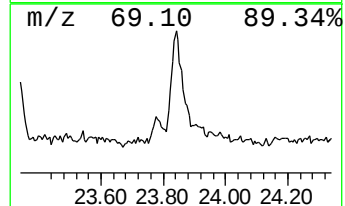
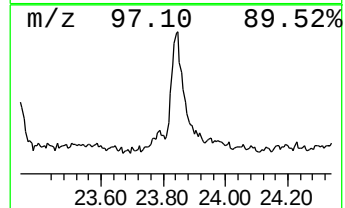
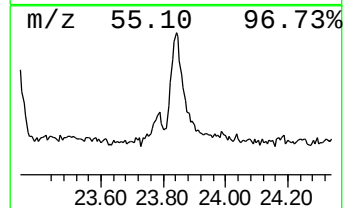
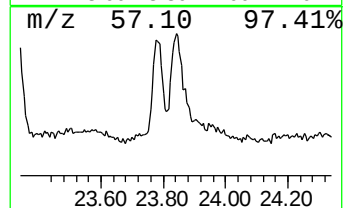
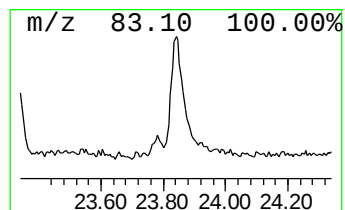
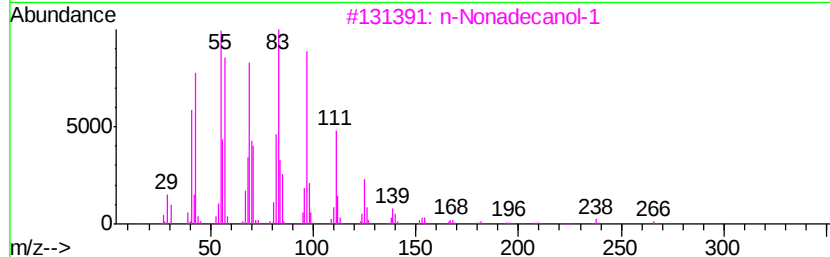
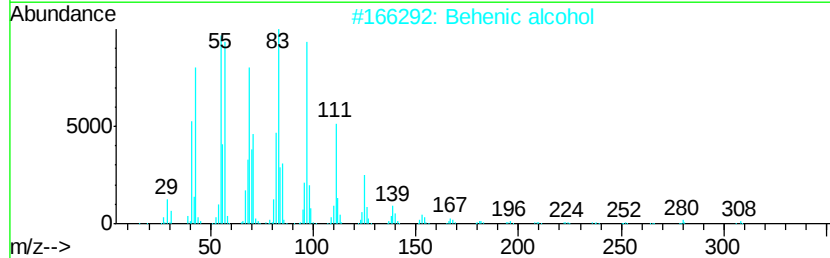
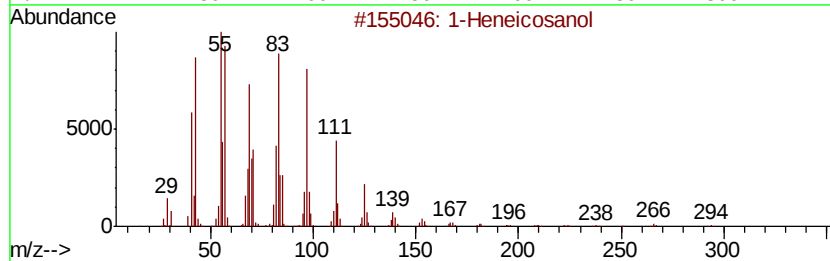
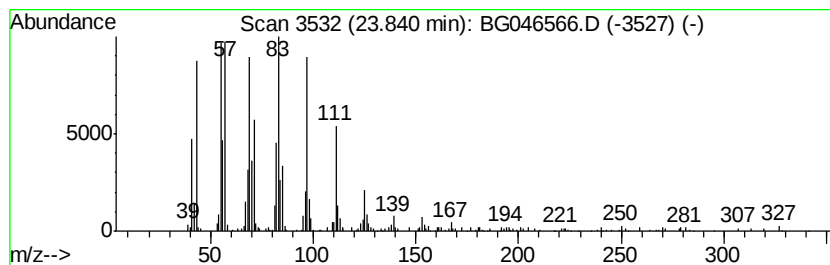
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.		
23.84	5.07 ng	324574	Perylene-d12		24.65		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	94
2			Behenic alcohol	326	C22H46O	000661-19-8	94
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5			1-Heptacosanol	396	C27H56O	002004-39-9	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG090820\
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 Acq On : 8 Sep 2020 20:37
 Operator : CG/JU
 Sample : L3919-17
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 TP-15

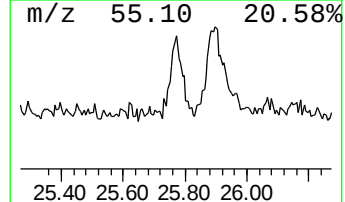
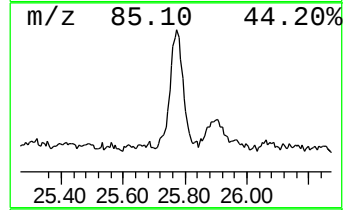
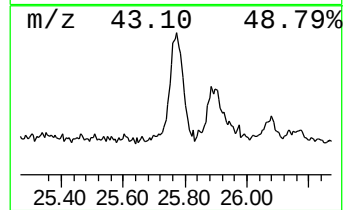
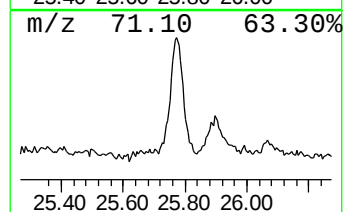
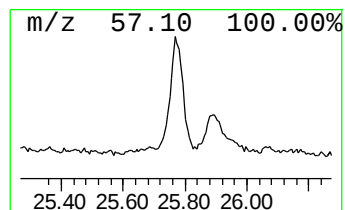
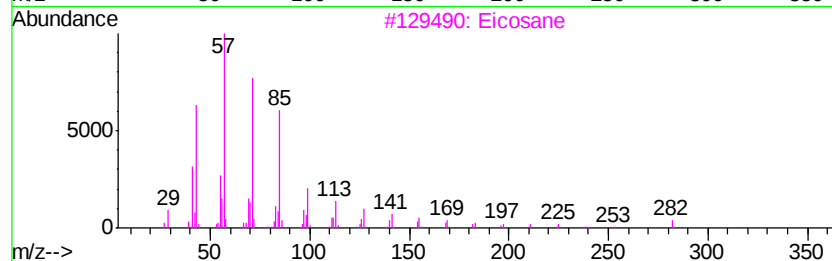
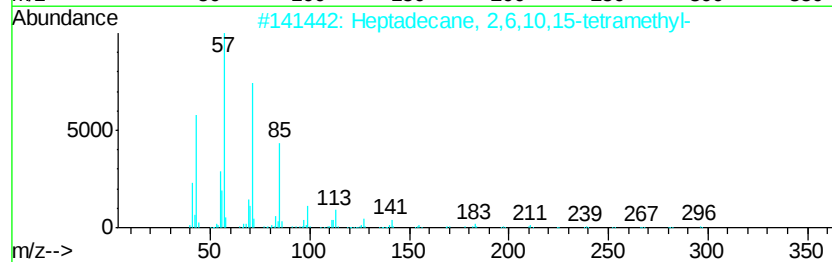
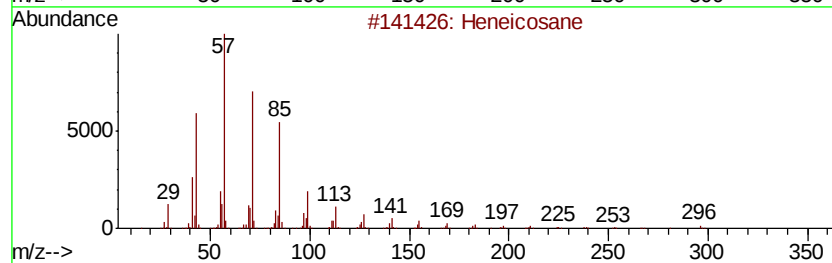
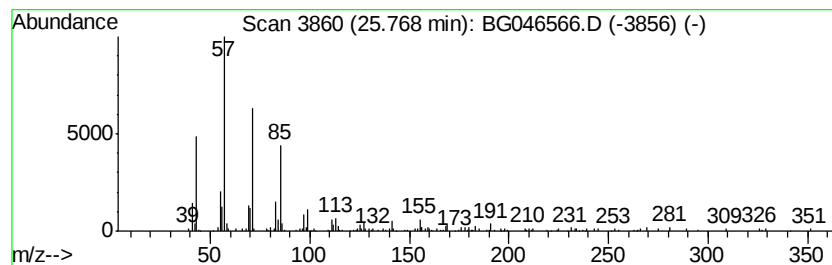
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 10 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.77	3.73 ng	239195	Perylene-d12	24.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	89
3	Eicosane		282	C20H42	000112-95-8	87
4	Tetradecane, 2,6,10-trimethyl-		240	C17H36	014905-56-7	87
5	2-methyloctacosane		408	C29H60	1000376-72-8	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG090820\
 Data File : BG046566.D
 Acq On : 8 Sep 2020 20:37
 Operator : CG/JU
 Sample : L3919-17
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082520.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...	3.12	21.1	ng	423504	1	7.93	401438	20.0
n-Hexadecanoic acid	18.21	3.1	ng	184699	4	17.30	1186540	20.0
unknown19.13	19.13	2.6	ng	152409	4	17.30	1186540	20.0
unknown20.46	20.46	4.8	ng	291827	5	21.55	1213480	20.0
1-Octadecene	21.21	9.8	ng	593067	5	21.55	1213480	20.0
4H-1-Benzopyran-4...	22.14	2.4	ng	145542	5	21.55	1213480	20.0
1-Heptacosanol	22.36	4.1	ng	249049	5	21.55	1213480	20.0
Oxirane, hexadecyl-	23.34	3.6	ng	232710	6	24.65	1281500	20.0
1-Heneicosanol	23.84	5.1	ng	324574	6	24.65	1281500	20.0
Heneicosane	25.77	3.7	ng	239195	6	24.65	1281500	20.0