

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
 Data File : BF109074.D
 Acq On : 18 Sep 2018 4:00
 Operator : JU/SJ
 Sample : J4943-03
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RBR200051

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_F\METHODS\8270-BF091418.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	4.925	436	440	451	rVB	207326	275887	9.75%	1.064%
2	5.342	506	511	514	rBV	2371553	2453080	86.72%	9.465%
3	6.360	679	684	687	rVB	2223386	2175014	76.89%	8.392%
4	6.489	702	706	710	rBV	2780905	2662684	94.13%	10.274%
5	6.719	742	745	749	rBV	872330	762402	26.95%	2.942%
6	6.878	768	772	775	rBV	2612585	2224316	78.64%	8.582%
7	7.278	836	840	843	rBV	1788919	1712191	60.53%	6.606%
8	7.507	876	879	883	rBV	87710	74887	2.65%	0.289%
9	8.001	959	963	966	rBV	1098270	871873	30.82%	3.364%
10	8.248	1000	1005	1013	rBV2	25429	45629	1.61%	0.176%
11	9.078	1142	1146	1149	rBV	3437319	2828630	100.00%	10.914%
12	9.466	1210	1212	1216	rBV	202013	177132	6.26%	0.683%
13	9.748	1257	1260	1264	rBV	966802	827643	29.26%	3.193%
14	10.089	1314	1318	1321	rBV2	39709	36250	1.28%	0.140%
15	10.536	1389	1394	1403	rBV	1676973	1604941	56.74%	6.192%
16	10.683	1413	1419	1423	rBV	45093	54533	1.93%	0.210%
17	11.148	1495	1498	1503	rVB2	30645	33792	1.19%	0.130%
18	11.224	1505	1511	1515	rVV	917172	883120	31.22%	3.407%
19	11.277	1518	1520	1528	rVB8	25638	45167	1.60%	0.174%
20	11.771	1600	1604	1612	rBV2	317272	331491	11.72%	1.279%
21	12.554	1734	1737	1740	rBV	65548	70205	2.48%	0.271%
22	12.813	1776	1781	1784	rBV	3092268	2797809	98.91%	10.795%
23	13.183	1841	1844	1847	rVB	45353	42651	1.51%	0.165%
24	13.718	1931	1935	1948	rVB	157612	212714	7.52%	0.821%
25	13.854	1954	1958	1961	rBV	1013579	956131	33.80%	3.689%
26	14.036	1986	1989	1996	rVB	37720	39817	1.41%	0.154%
27	14.342	2038	2041	2050	rBV	74462	77652	2.75%	0.300%
28	14.636	2088	2091	2095	rVB	109978	96709	3.42%	0.373%
29	14.707	2100	2103	2106	rVB	275851	256514	9.07%	0.990%
30	14.954	2141	2145	2150	rBV	144255	155715	5.50%	0.601%
31	15.254	2191	2196	2201	rBV	581035	647055	22.88%	2.497%
32	15.307	2201	2205	2212	rVB	119784	154723	5.47%	0.597%
33	15.495	2233	2237	2242	rVB6	26362	39742	1.40%	0.153%
34	15.712	2270	2274	2280	rBV	102792	133411	4.72%	0.515%

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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

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	16.177	2349	2353	2368	rVB2	50854	107668	3.81%	0.415%
36	16.442	2394	2398	2406	rVB8	25390	48376	1.71%	0.187%

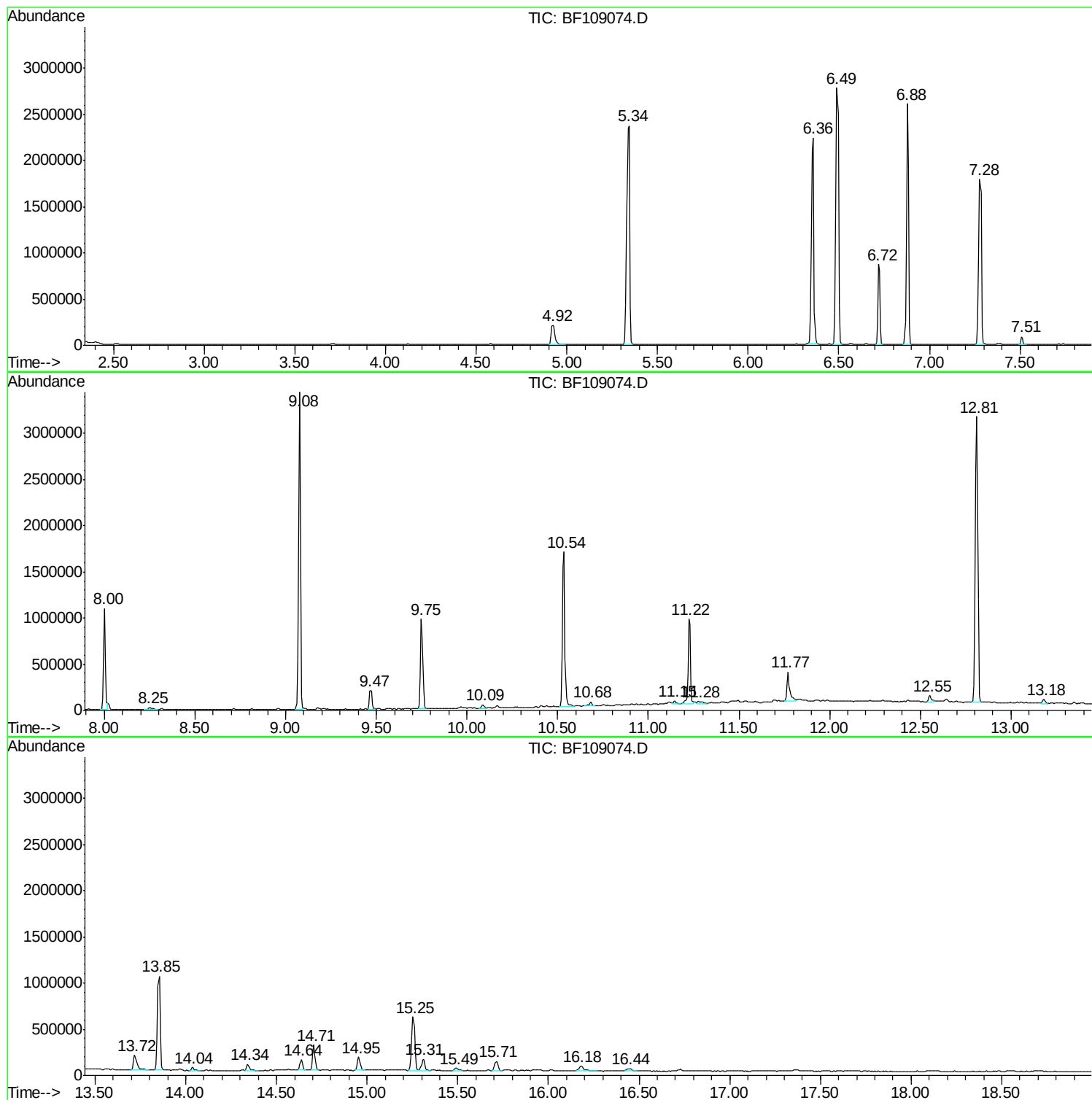
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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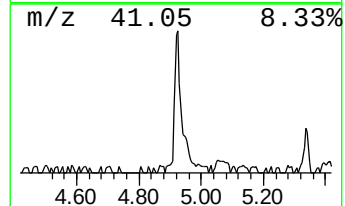
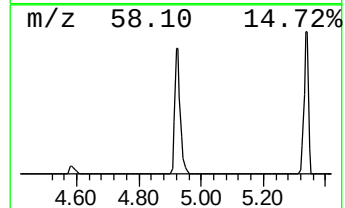
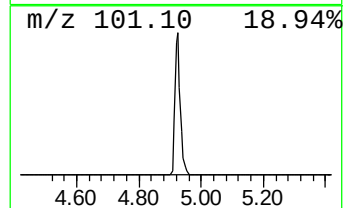
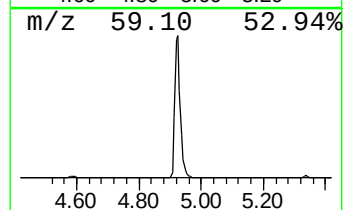
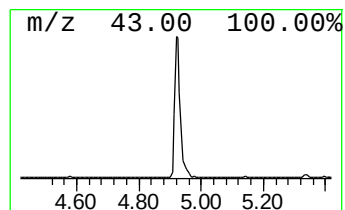
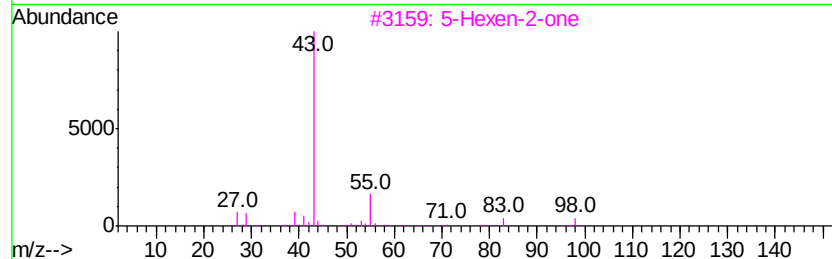
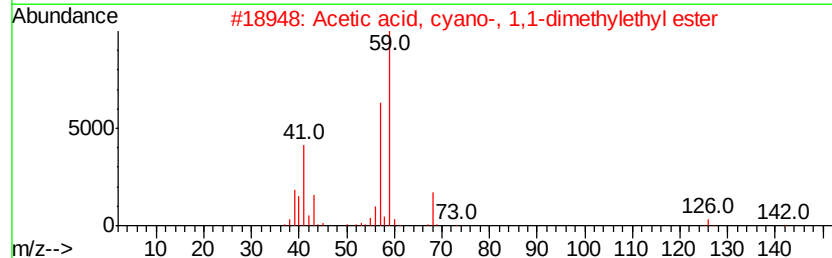
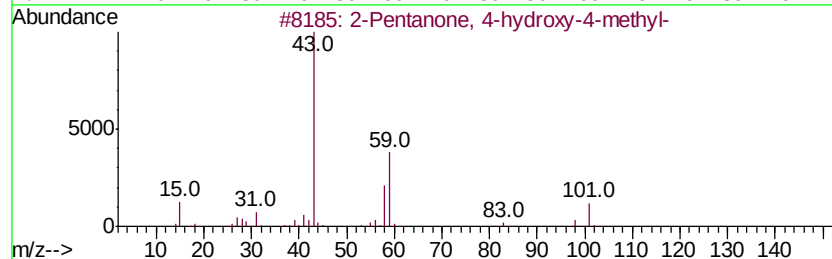
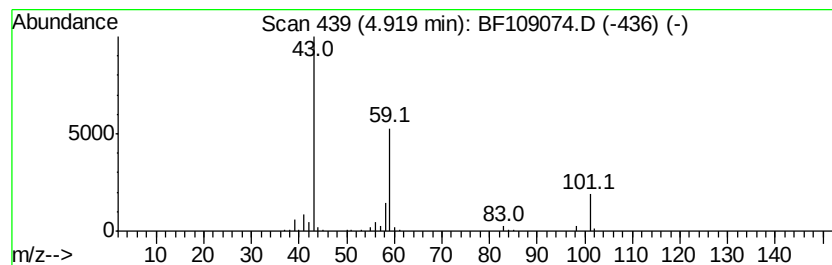
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	7.24 ng	275887	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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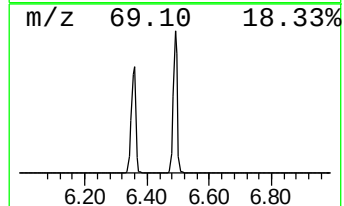
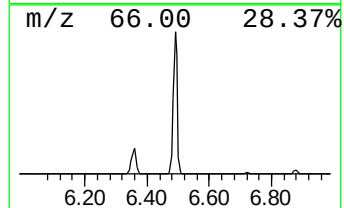
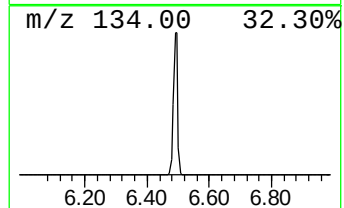
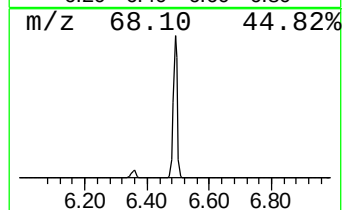
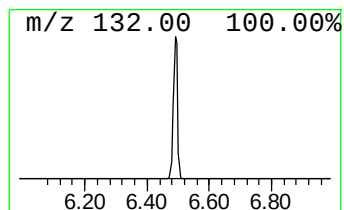
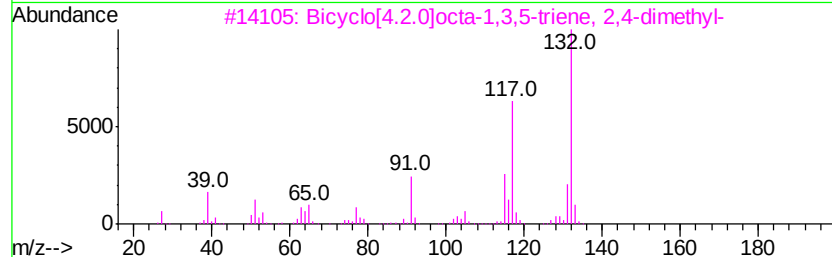
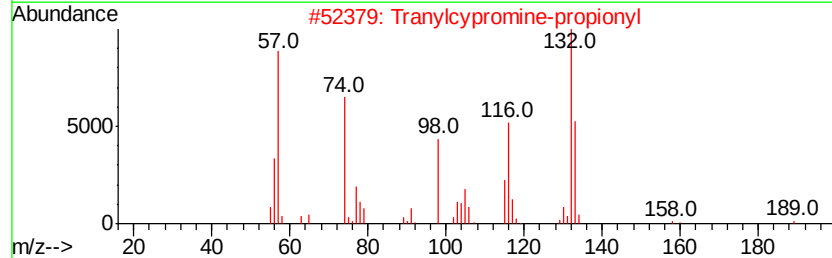
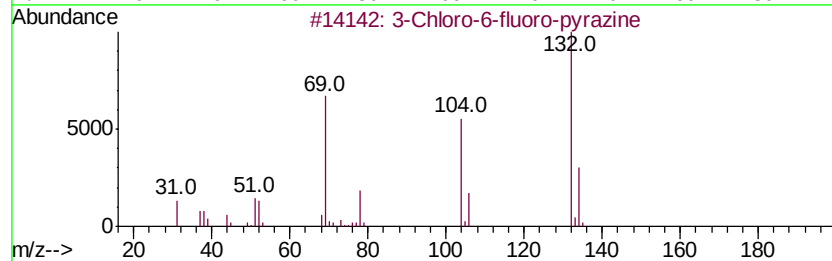
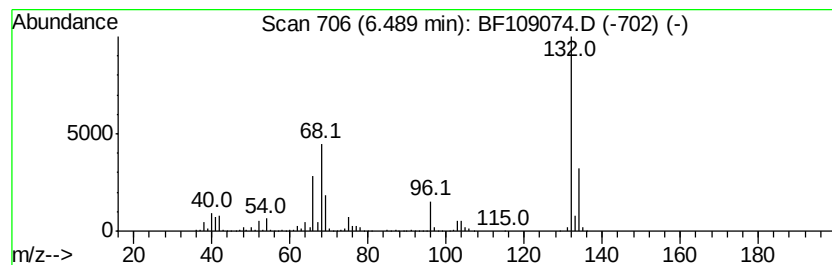
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	69.85 ng	2662680	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
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		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		5-Aminoindole	132	C8H8N2	005192-03-0	9



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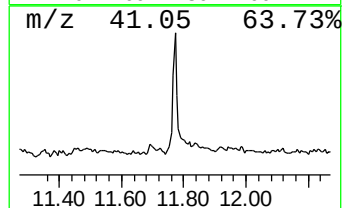
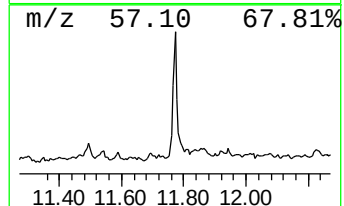
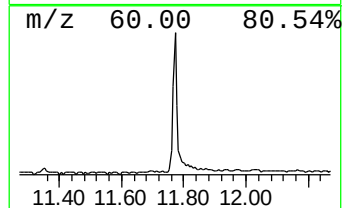
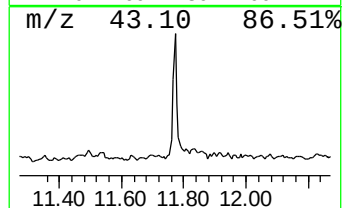
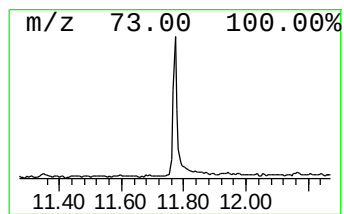
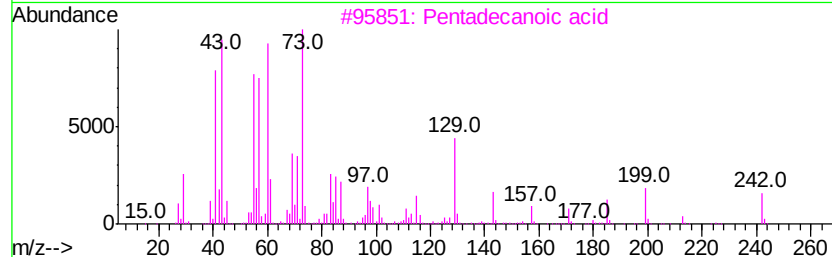
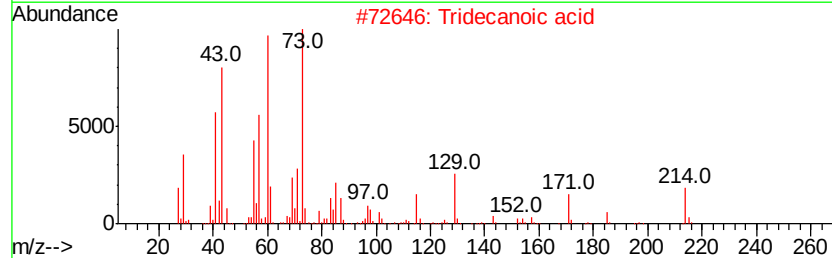
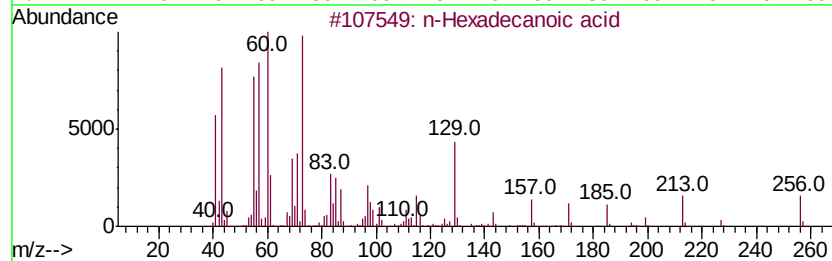
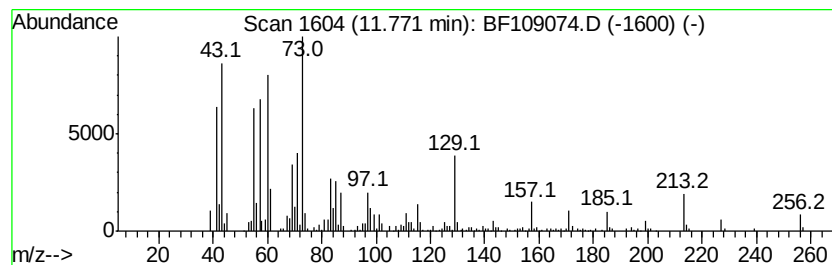
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	7.51 ng	331491	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68



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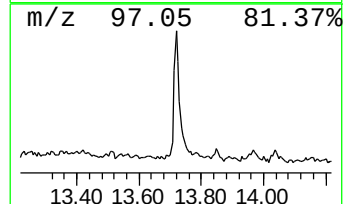
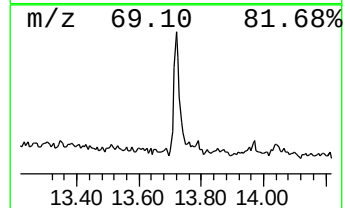
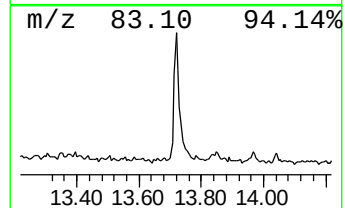
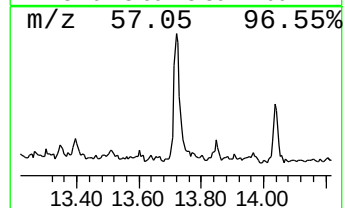
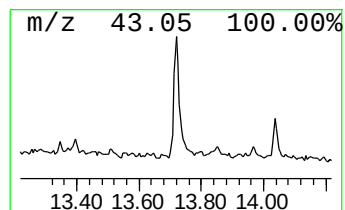
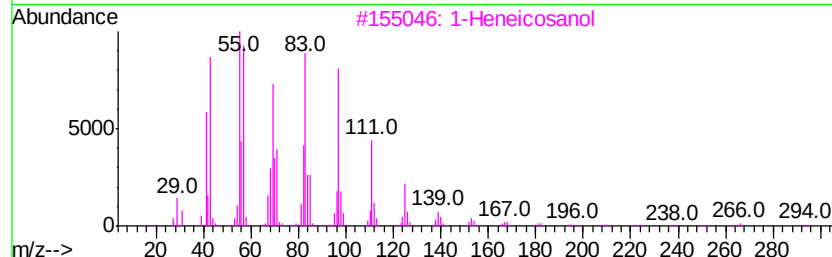
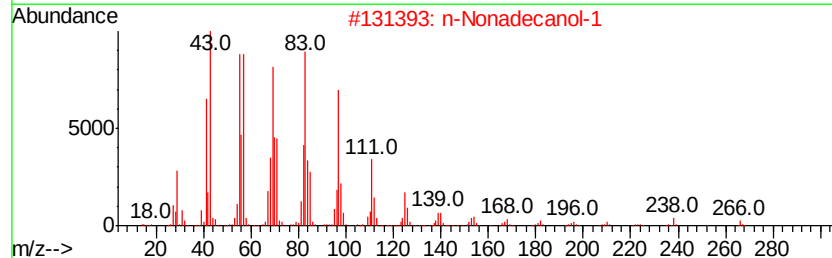
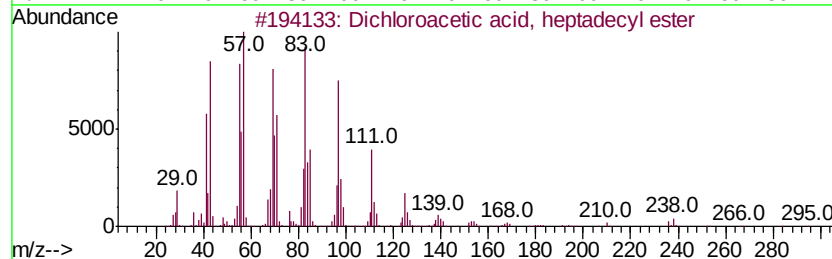
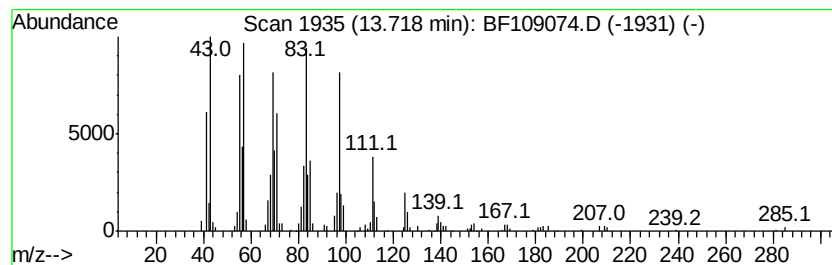
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Dichloroacetic acid, heptad... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	4.45 ng	212714	Chrysene-d12	13.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3		1-Heneicosanol	312	C21H44O	015594-90-8	94
4		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



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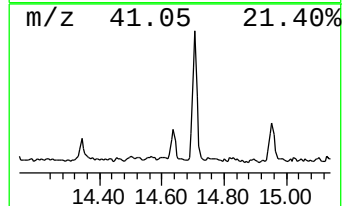
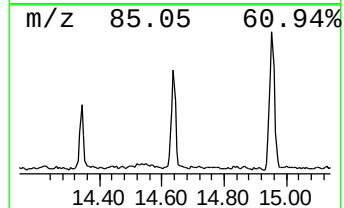
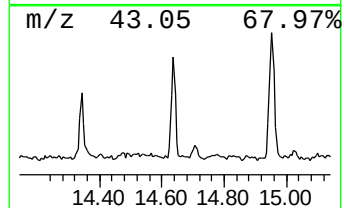
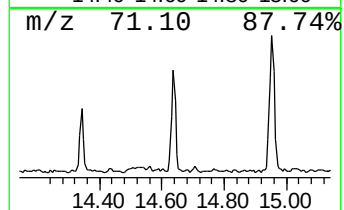
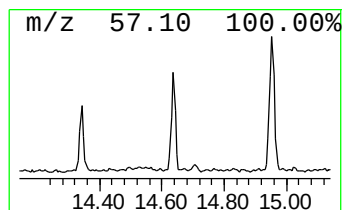
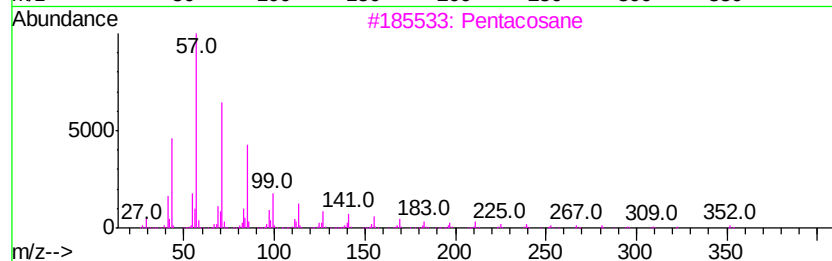
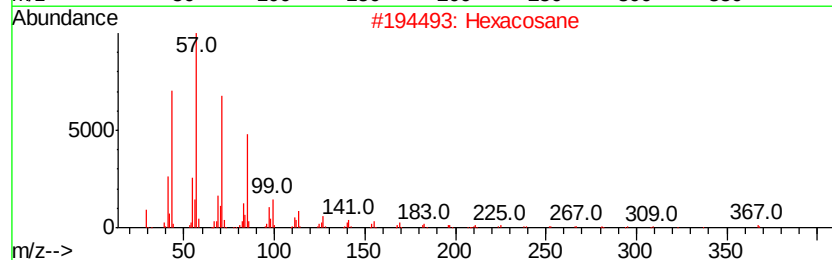
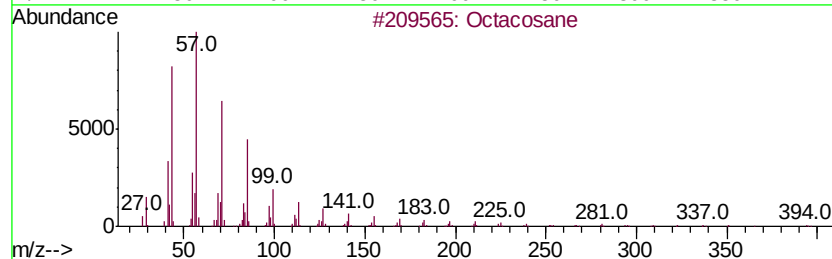
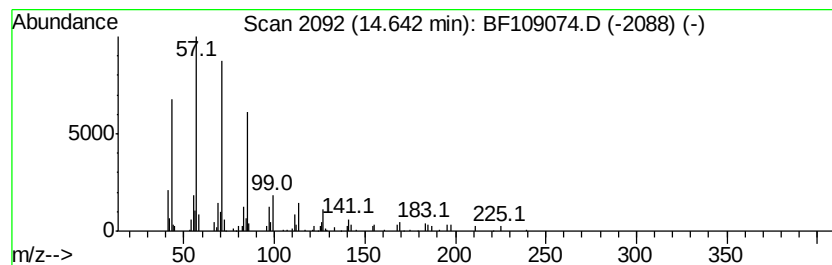
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Peak Number 6 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.99 ng	96709	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Pentacosane	352	C25H52	000629-99-2	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Tetratetracontane	619	C44H90	007098-22-8	91



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Instrument :
BNA_F
ClientSampleId :
RBR200051

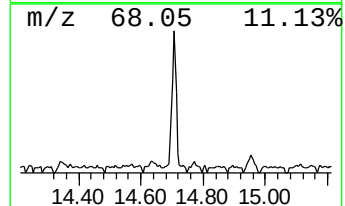
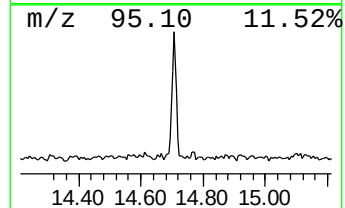
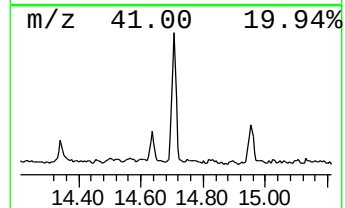
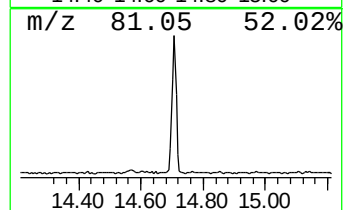
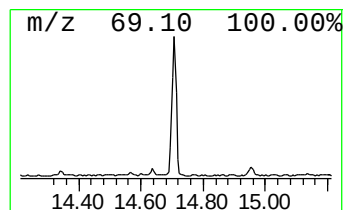
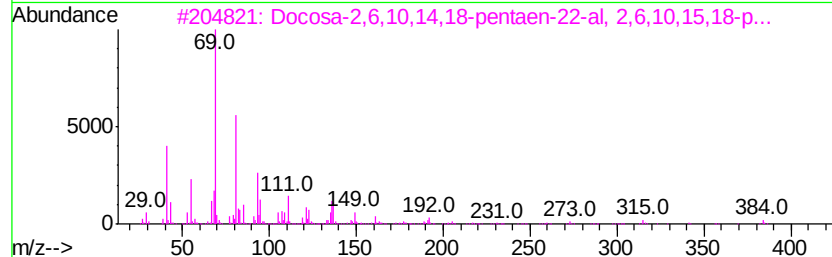
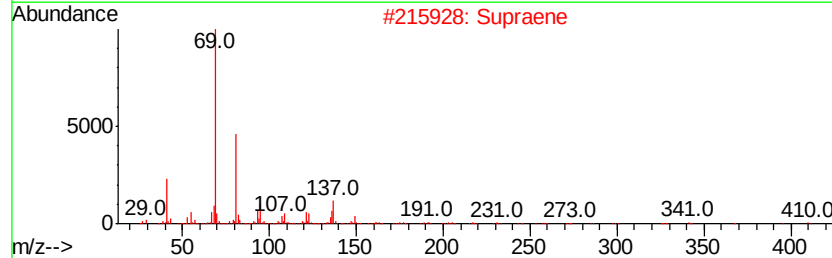
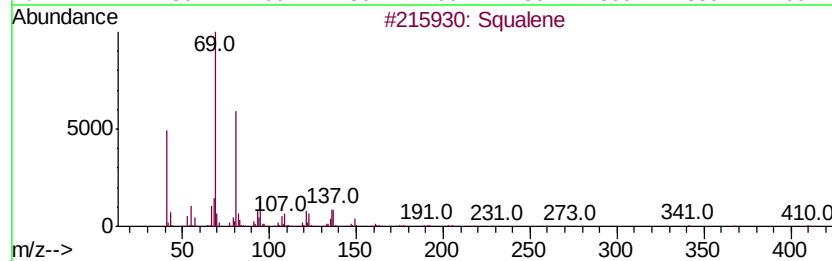
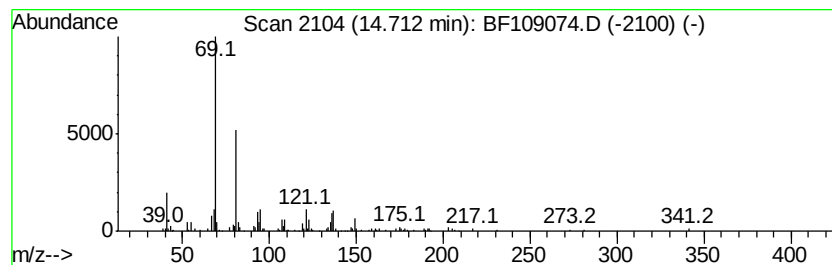
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	7.93 ng	256514	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	87
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109074.D
Acq On : 18 Sep 2018 4:00
Operator : JU/SJ
Sample : J4943-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

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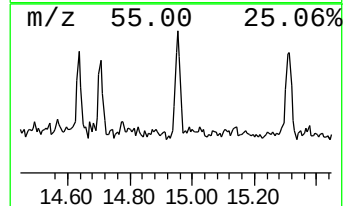
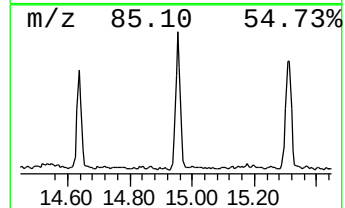
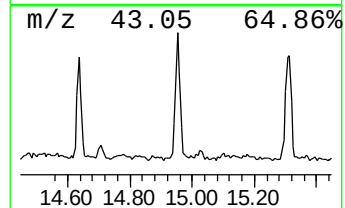
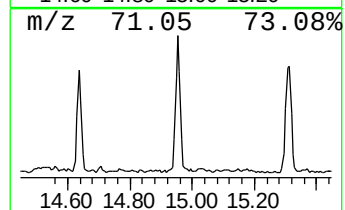
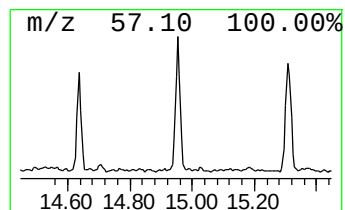
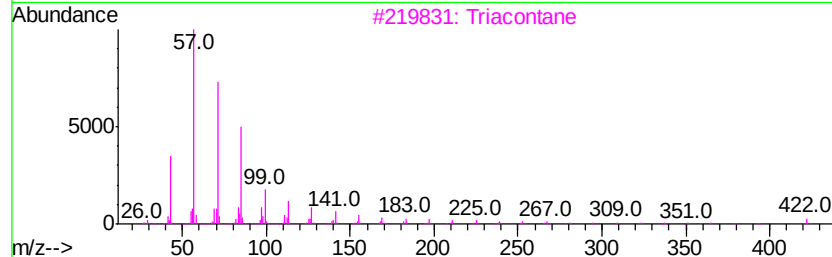
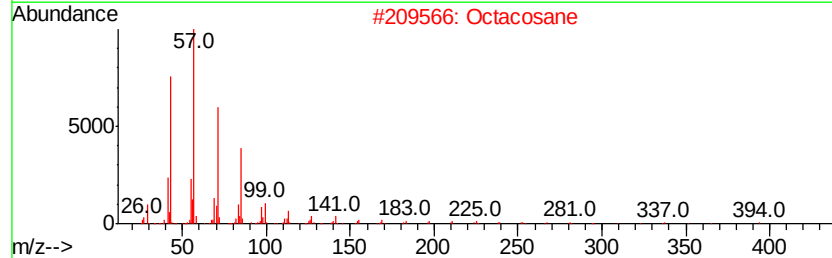
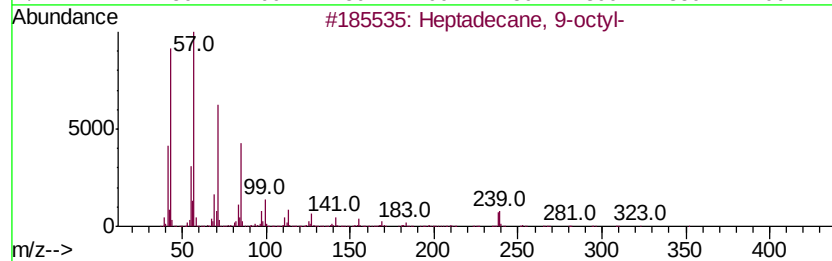
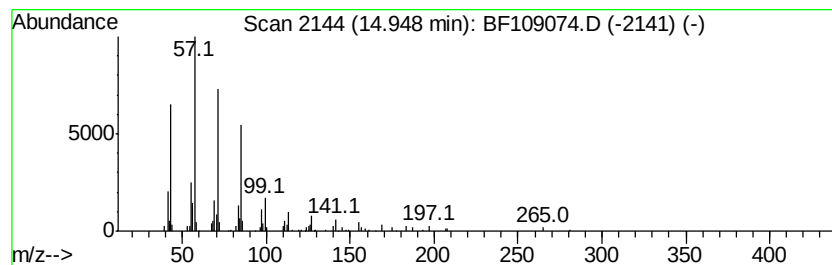
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	4.81 ng	155715	Perylene-d12	15.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
2	Octacosane		394	C28H58	000630-02-4	91
3	triacontane		422	C30H62	000638-68-6	91
4	Heptadecane		240	C17H36	000629-78-7	90
5	Heneicosane		296	C21H44	000629-94-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109074.D
Acq On : 18 Sep 2018 4:00
Operator : JU/SJ
Sample : J4943-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

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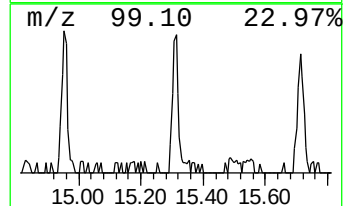
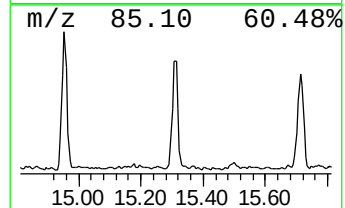
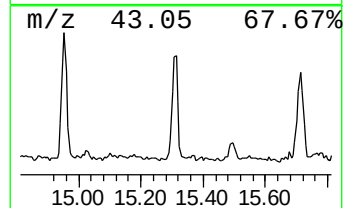
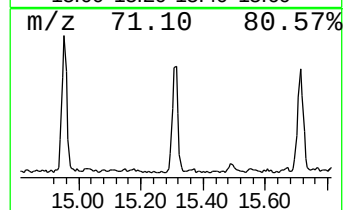
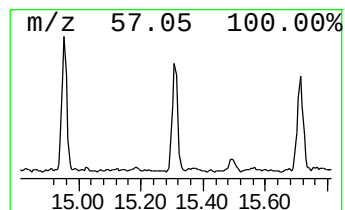
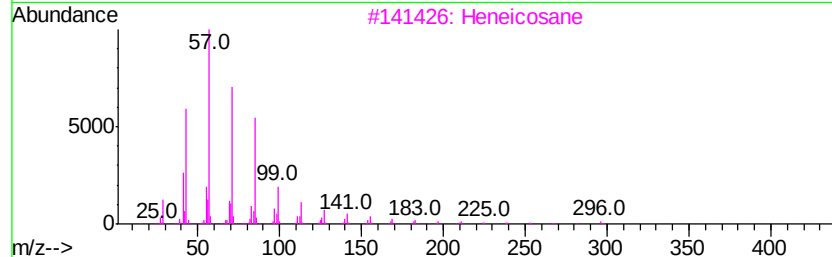
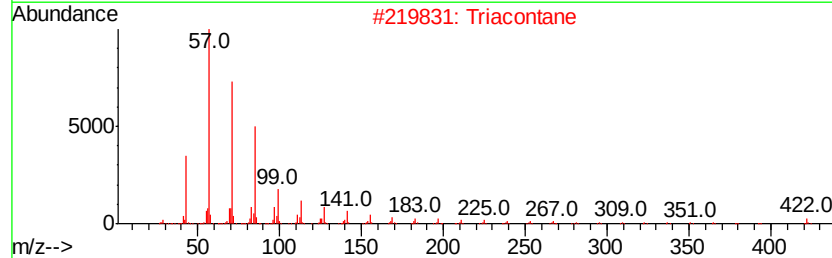
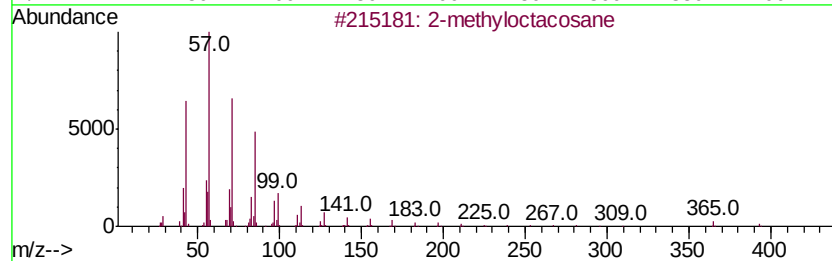
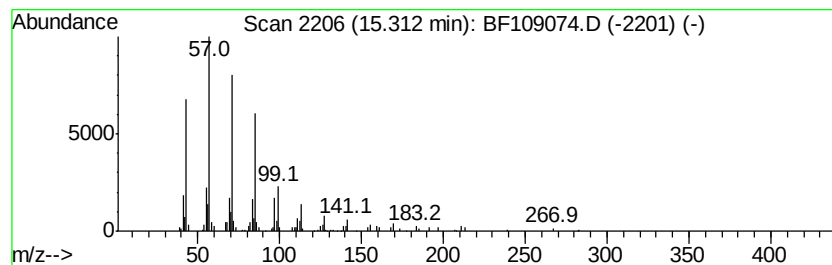
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	4.78 ng	154723	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Triacontane	422	C30H62	000638-68-6	91
3		Heneicosane	296	C21H44	000629-94-7	90
4		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5		Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109074.D
Acq On : 18 Sep 2018 4:00
Operator : JU/SJ
Sample : J4943-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

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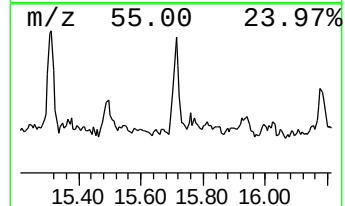
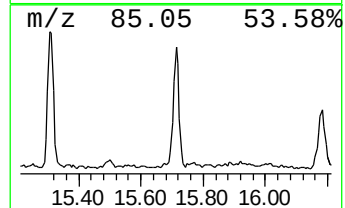
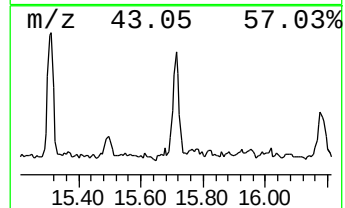
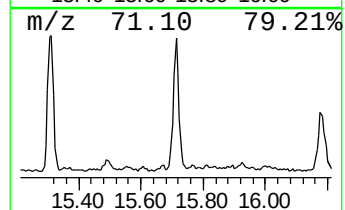
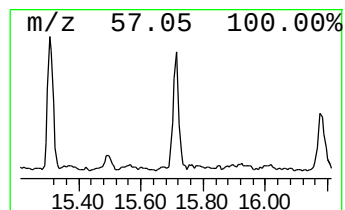
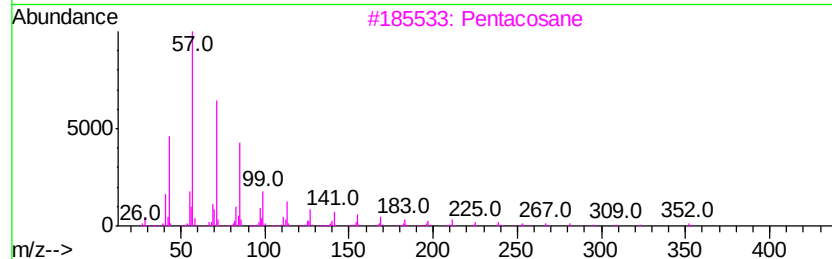
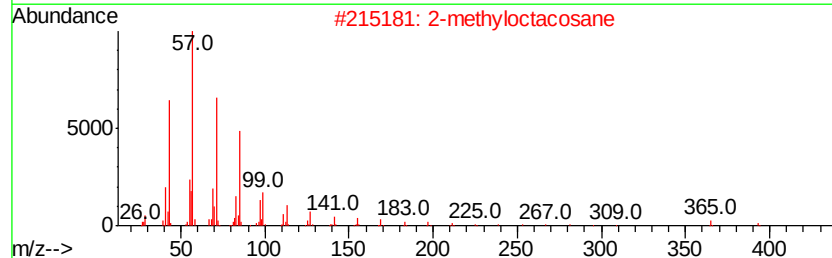
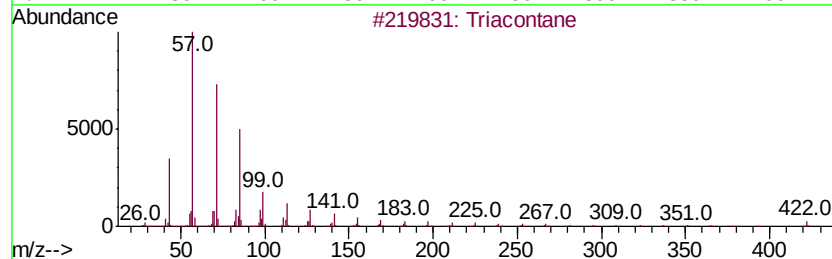
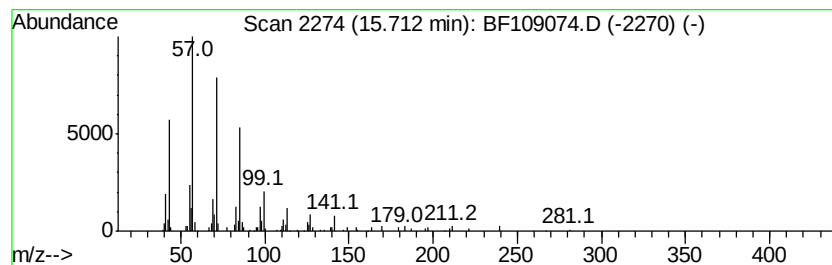
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Triacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	4.12 ng	133411	Perylene-d12	15.25

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane	422	C30H62	000638-68-6	91
2			2-methyloctacosane	408	C29H60	1000376-72-8	91
3			Pentacosane	352	C25H52	000629-99-2	91
4			Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	90
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091718\
Data File : BF109074.D
Acq On : 18 Sep 2018 4:00
Operator : JU/SJ
Sample : J4943-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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
2-Pentanone, 4-hy...	4.92	7.2	ng	275887	1	6.72	762402	20.0
unknown6.49	6.49	69.8	ng	2662680	1	6.72	762402	20.0
n-Hexadecanoic acid	11.77	7.5	ng	331491	4	11.22	883120	20.0
Dichloroacetic ac...	13.72	4.5	ng	212714	5	13.85	956131	20.0
Octacosane	14.64	3.0	ng	96709	6	15.25	647055	20.0
Squalene	14.71	7.9	ng	256514	6	15.25	647055	20.0
Heptadecane, 9-oc...	14.95	4.8	ng	155715	6	15.25	647055	20.0
2-methyloctacosane	15.31	4.8	ng	154723	6	15.25	647055	20.0
Triacontane	15.71	4.1	ng	133411	6	15.25	647055	20.0