

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
 Data File : BF109427.D
 Acq On : 28 Sep 2018 11:24
 Operator : JU/SJ
 Sample : J5133-07
 Misc :
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 092618-DBRI-F-D-B

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-BF092218.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	4.887	472	476	493	rVB	54708	66028	2.21%	0.357%
2	5.310	544	548	562	rBV	853725	762804	25.58%	4.122%
3	6.340	719	723	735	rBV2	517703	594353	19.93%	3.212%
4	6.475	742	746	749	rBV	1766487	1494248	50.12%	8.075%
5	6.704	782	785	789	rBV	732855	584431	19.60%	3.158%
6	6.863	808	812	815	rBV	2446638	2075319	69.61%	11.216%
7	7.269	876	881	884	rBV	1878472	1661043	55.71%	8.977%
8	7.986	999	1003	1010	rBV	910531	711646	23.87%	3.846%
9	9.063	1182	1186	1189	rBV	3276025	2981553	100.00%	16.113%
10	9.457	1250	1253	1265	rVB	127228	119177	4.00%	0.644%
11	9.733	1297	1300	1309	rVB2	862953	764713	25.65%	4.133%
12	10.516	1430	1433	1443	rBV	1059029	1037431	34.79%	5.607%
13	11.210	1548	1551	1555	rBV	778389	651235	21.84%	3.519%
14	12.792	1816	1820	1824	rBV	2336958	2237266	75.04%	12.091%
15	13.704	1972	1975	1977	rBV2	43632	46355	1.55%	0.251%
16	13.733	1977	1980	1994	rVB6	32899	86752	2.91%	0.469%
17	13.839	1994	1998	2001	rBV	747357	665572	22.32%	3.597%
18	14.021	2025	2029	2032	rBV	71950	62004	2.08%	0.335%
19	14.321	2077	2080	2084	rBV	113091	98543	3.31%	0.533%
20	14.592	2122	2126	2128	rBV	51455	53802	1.80%	0.291%
21	14.615	2128	2130	2135	rVV	163947	150322	5.04%	0.812%
22	14.686	2138	2142	2146	rVV	454797	396737	13.31%	2.144%
23	14.933	2179	2184	2189	rBV	170822	185308	6.22%	1.001%
24	15.239	2231	2236	2240	rBV	453922	515343	17.28%	2.785%
25	15.286	2240	2244	2249	rVB	155733	193043	6.47%	1.043%
26	15.680	2306	2311	2319	rBV	119075	164762	5.53%	0.890%
27	16.145	2385	2390	2399	rVB	59984	102457	3.44%	0.554%
28	16.680	2475	2481	2490	rBV2	21094	41586	1.39%	0.225%

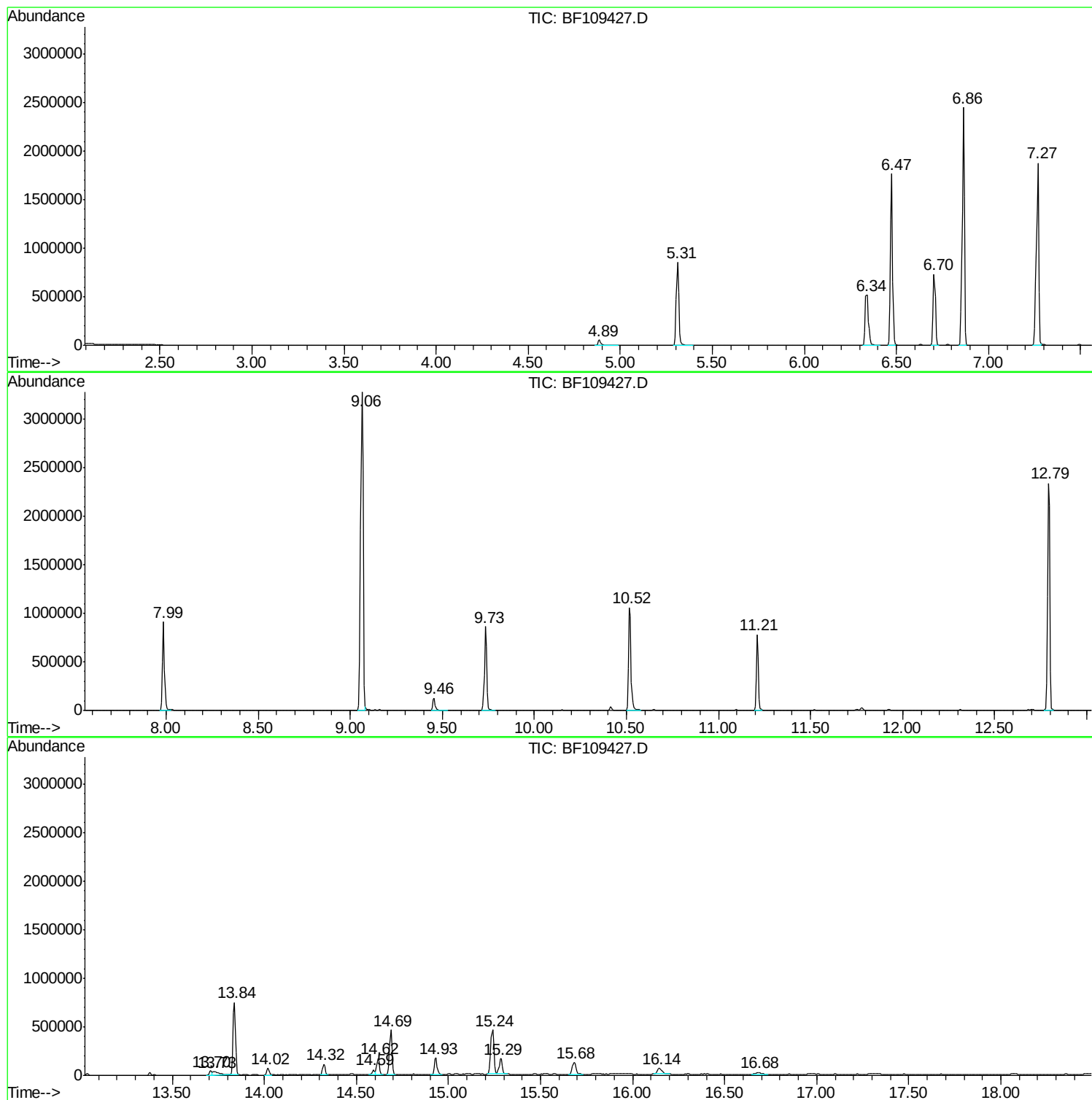
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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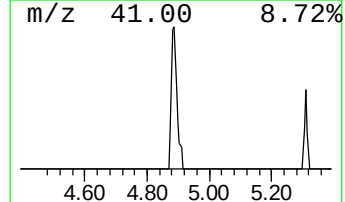
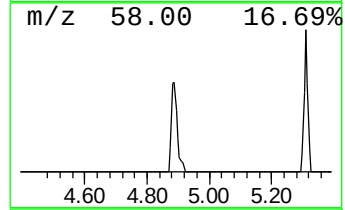
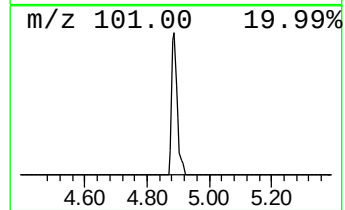
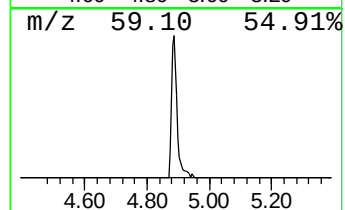
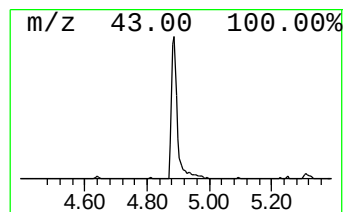
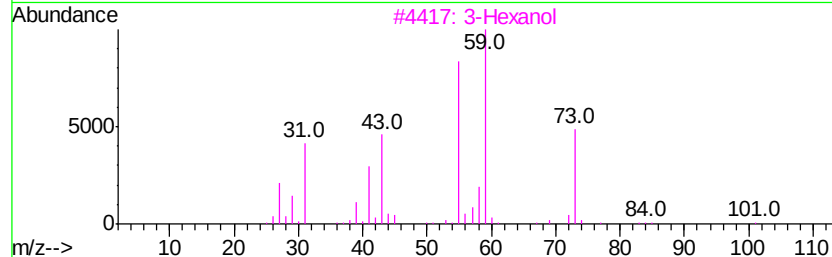
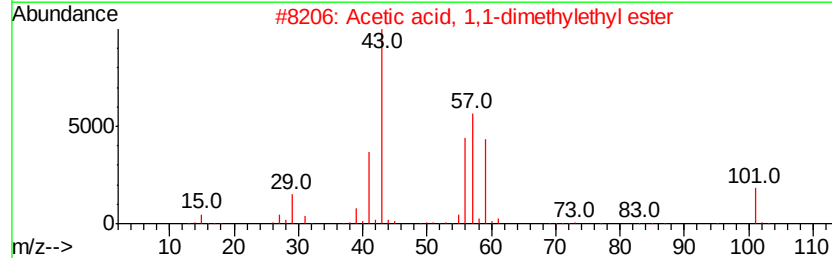
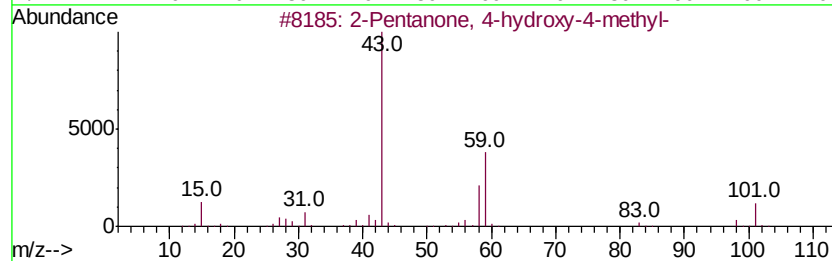
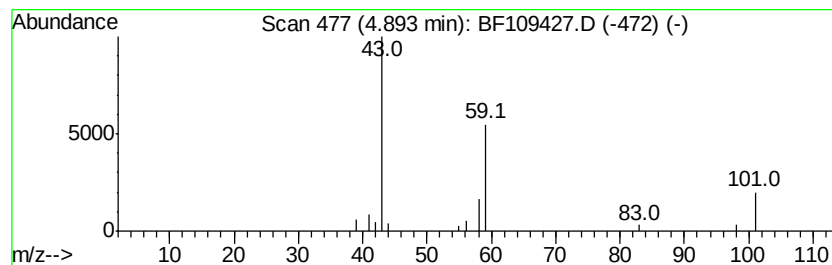
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	2.26 ng	66028	1,4-Dichlorobenzene-d4	6.70

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			3-Hexanol	102	C6H14O	000623-37-0	33
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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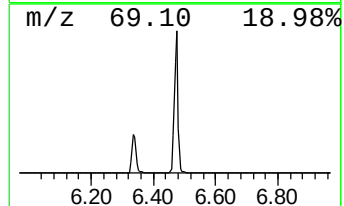
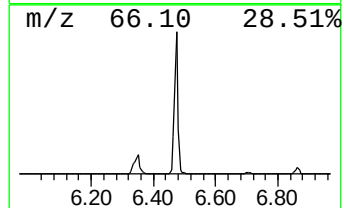
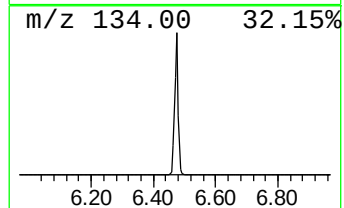
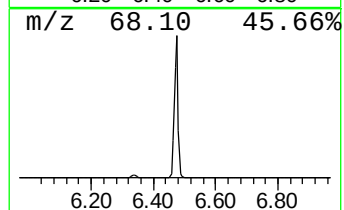
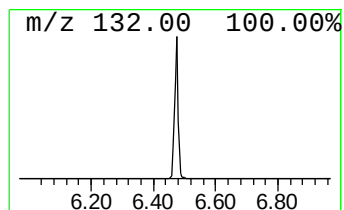
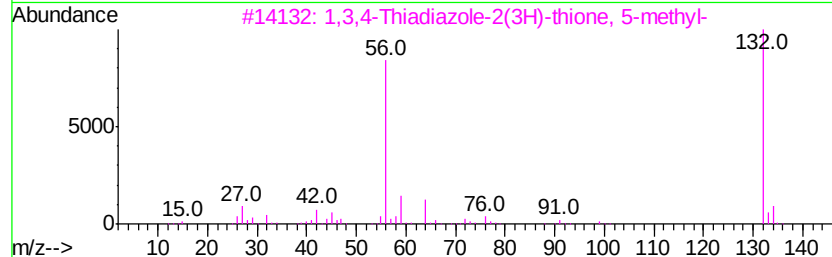
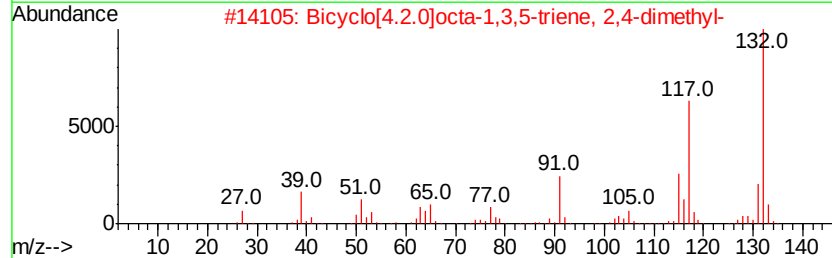
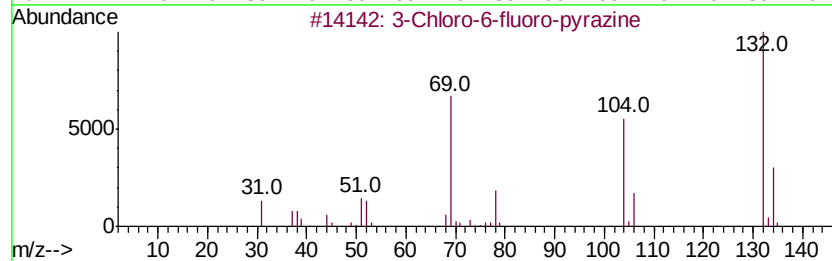
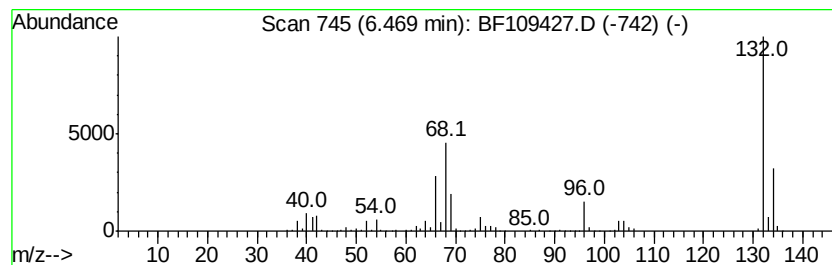
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Peak Number 2 unknown6.47 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	51.14 ng	1494250	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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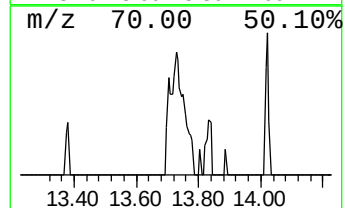
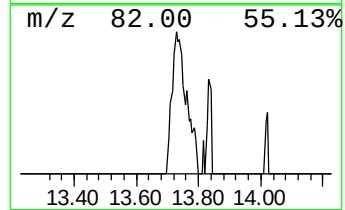
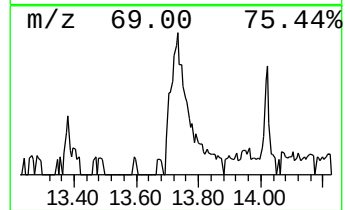
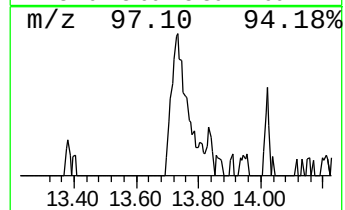
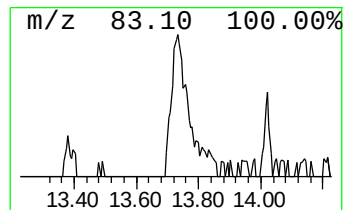
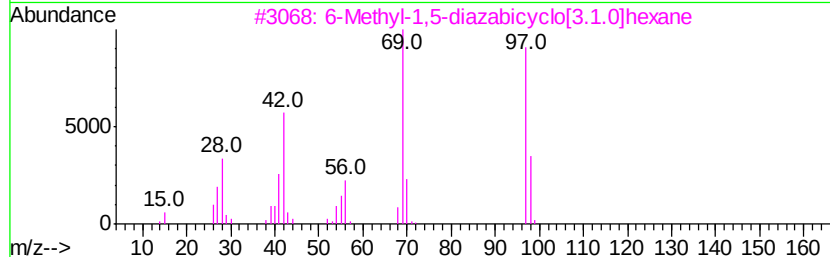
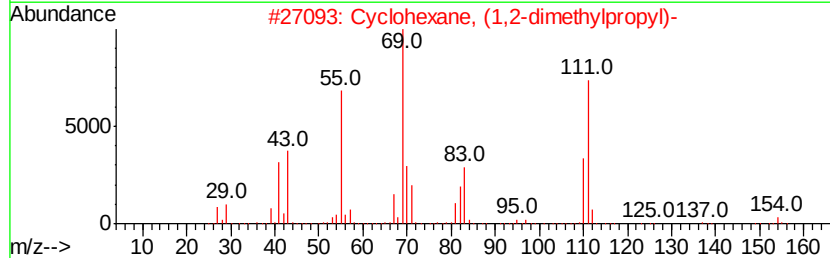
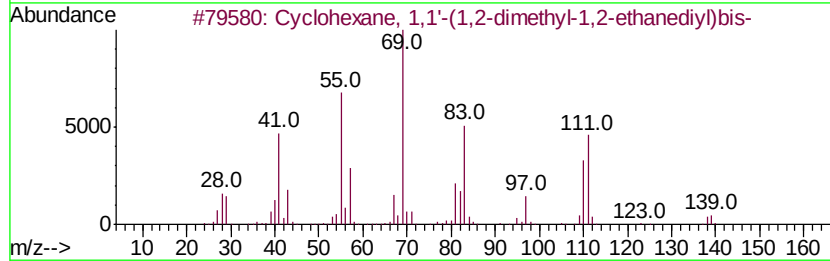
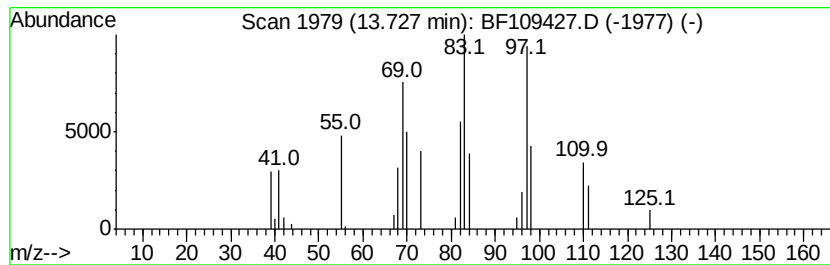
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Peak Number 4 unknown13.73 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	2.61 ng	86752	Chrysene-d12	13.84

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, 1,1'-(1,2-dimethyl-...	222	C16H30	074663-71-1	38
2		Cyclohexane, (1,2-dimethylpropyl)-	154	C11H22	051284-29-8	35
3		6-Methyl-1,5-diazabicyclo[3.1.0]...	98	C5H10N2	100463-00-1	27
4		Cyclopentane, 1,1,3,4-tetramethy...	126	C9H18	053907-60-1	23
5		2-Thiopheneacetic acid, 2-ethylc...	252	C14H20O2S	1000278-96-1	23



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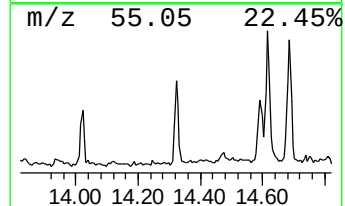
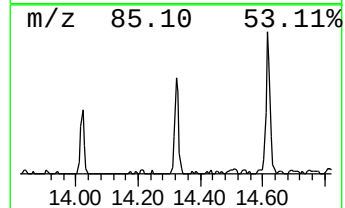
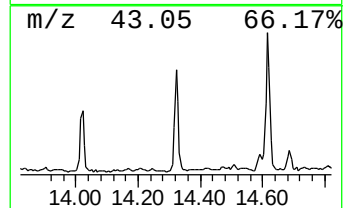
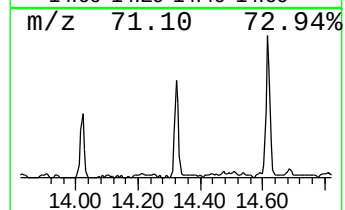
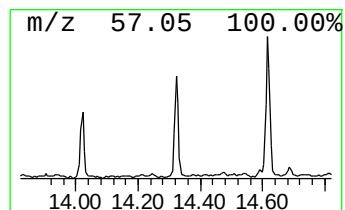
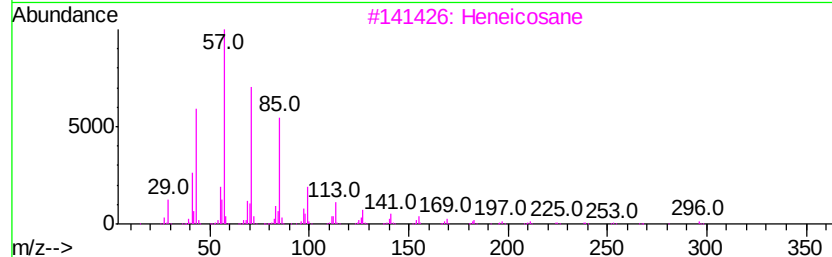
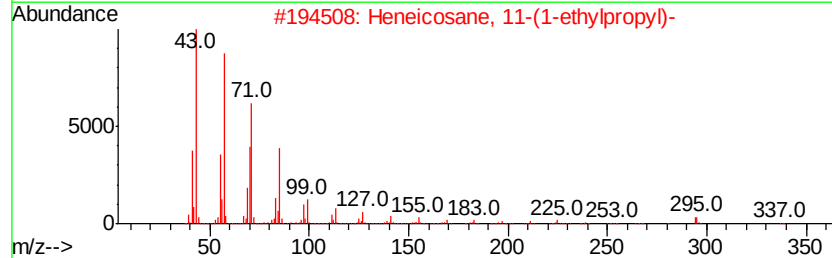
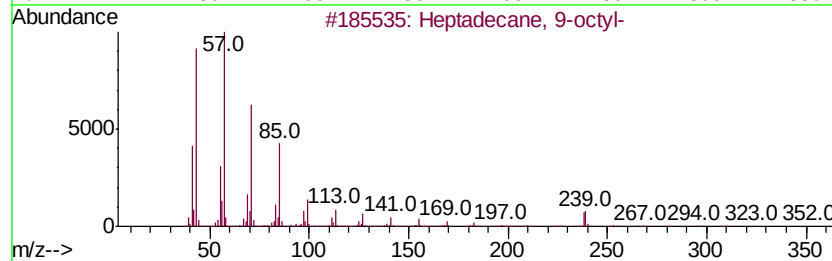
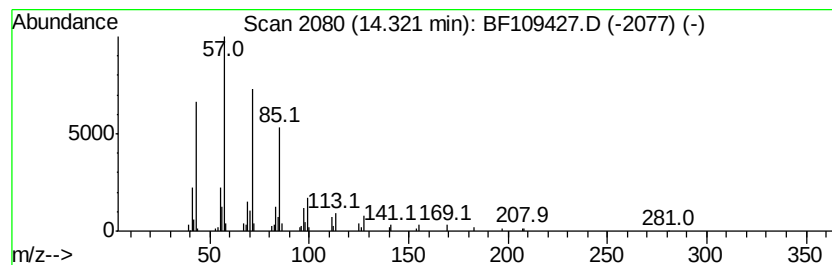
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Peak Number 5 Heptadecane, 9-octyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.32	2.96 ng	98543	Chrysene-d12	13.84	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
2	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
3	Heneicosane	296	C21H44	000629-94-7	86
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	83
5	Octacosane	394	C28H58	000630-02-4	76



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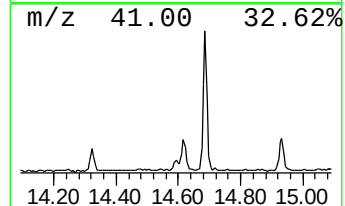
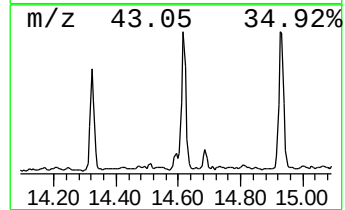
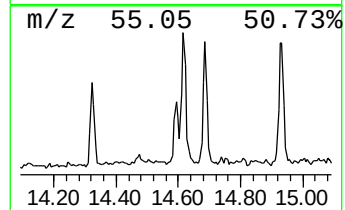
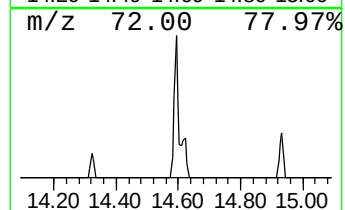
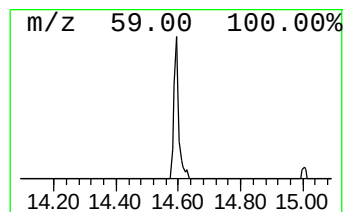
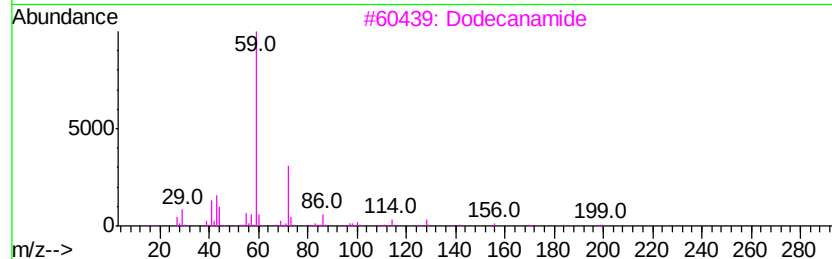
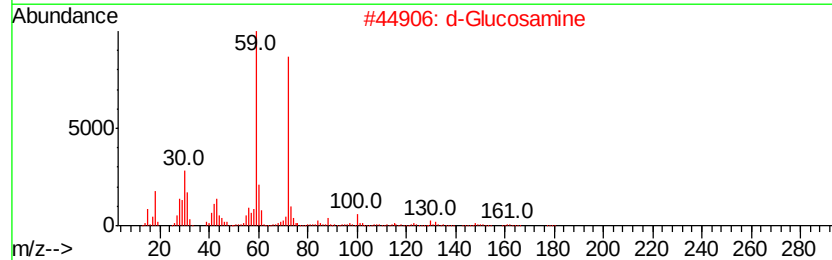
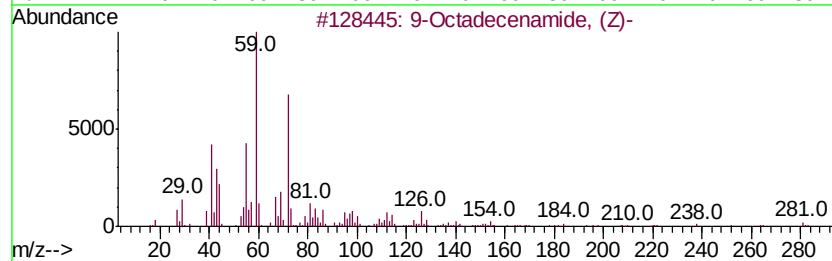
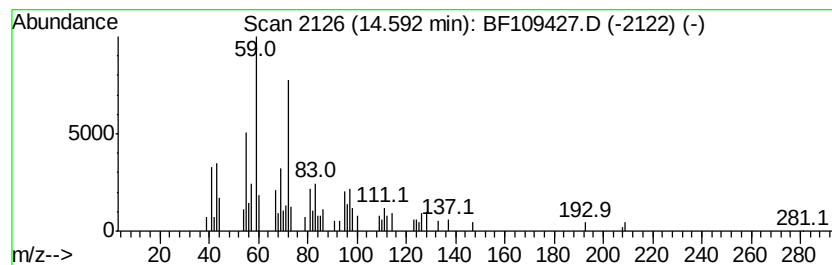
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	2.09 ng	53802	Perylene-d12	15.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	59
2		d-Glucosamine	179	C6H13NO5	000090-77-7	47
3		Dodecanamide	199	C12H25NO	001120-16-7	43
4		7-Nonenamide	155	C9H17NO	090949-53-4	38
5		3-Tetradecanol	214	C14H30O	001653-32-3	35



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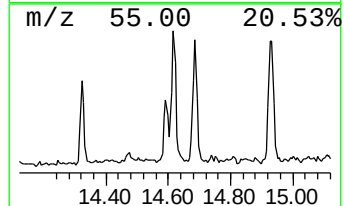
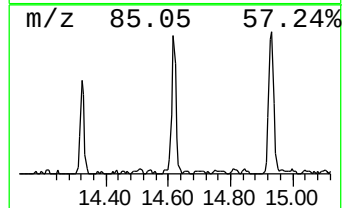
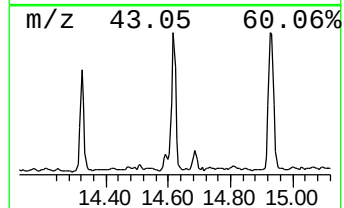
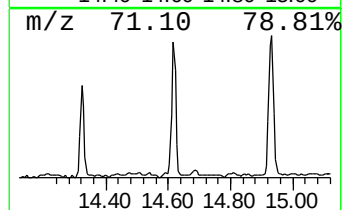
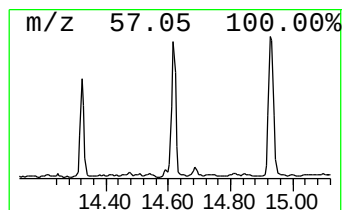
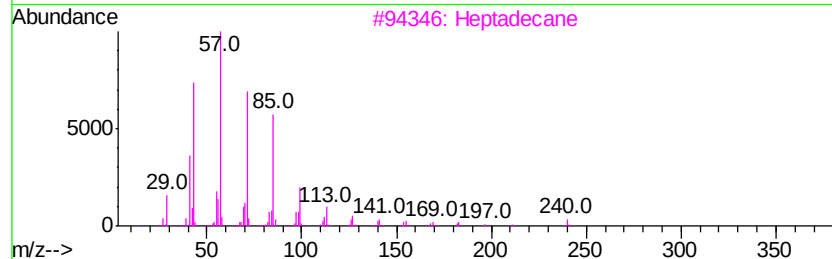
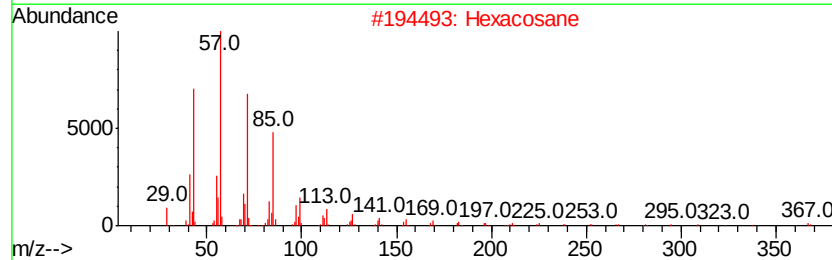
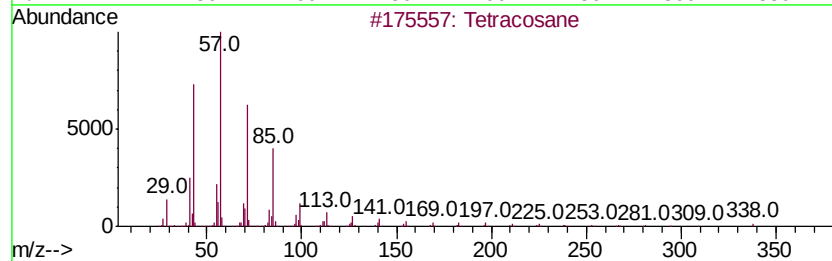
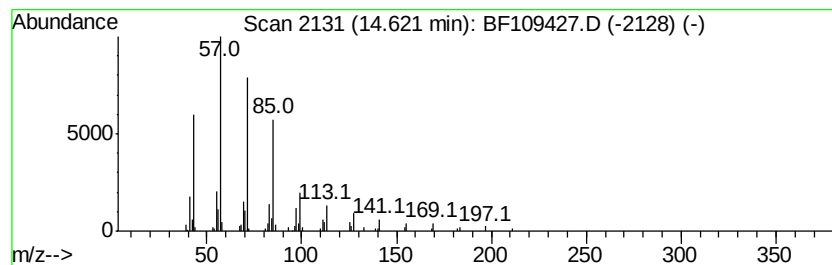
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	5.83 ng	150322	Perylene-d12	15.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heptadecane	240	C17H36	000629-78-7	91
4		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
Data File : BF109427.D
Acq On : 28 Sep 2018 11:24
Operator : JU/SJ
Sample : J5133-07
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
092618-DBRI-F-D-B

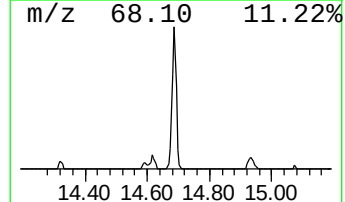
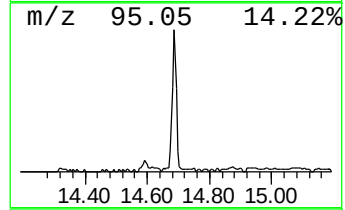
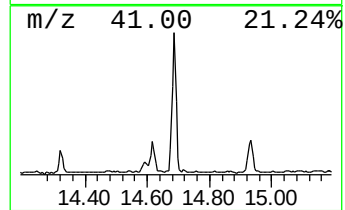
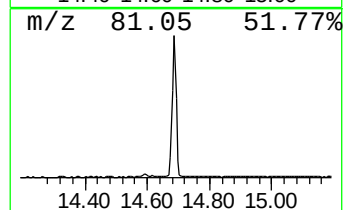
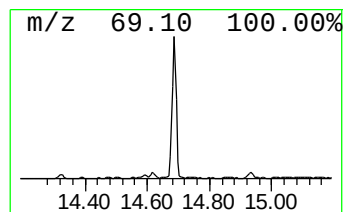
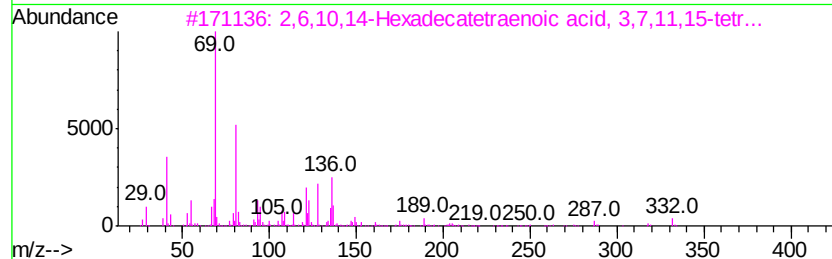
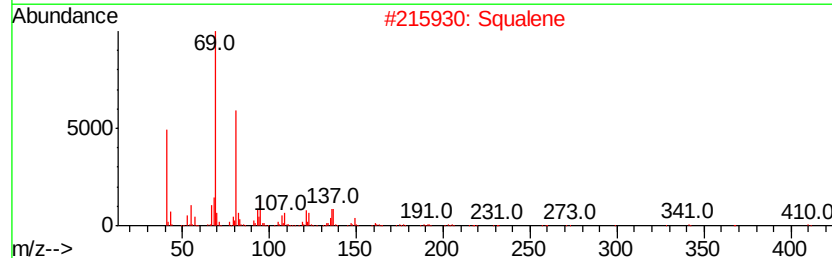
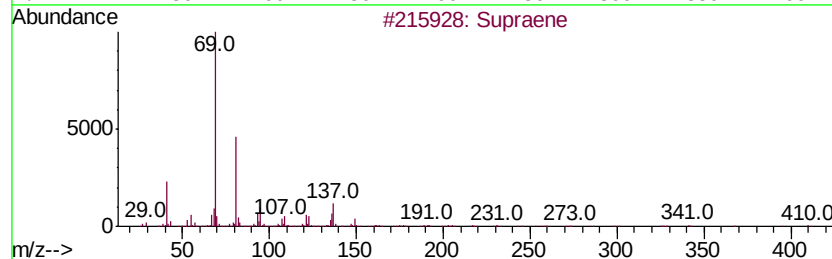
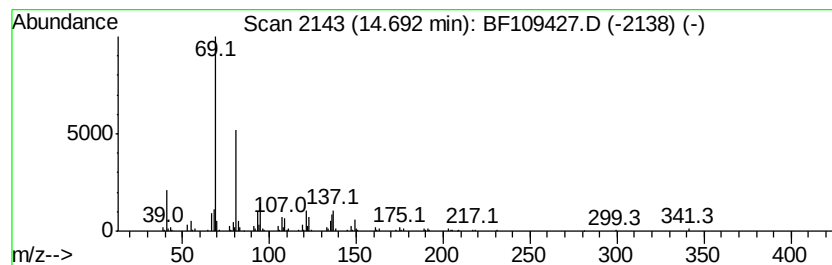
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	15.40 ng	396737	Perylene-d12	15.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
4		(.+/-)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	64
5		1,6,10,14-Hexadecatetraen-3-ol, ...	290	C20H34O	001113-21-9	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
Data File : BF109427.D
Acq On : 28 Sep 2018 11:24
Operator : JU/SJ
Sample : J5133-07
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
092618-DBRI-F-D-B

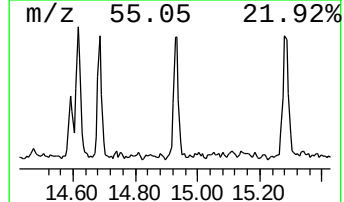
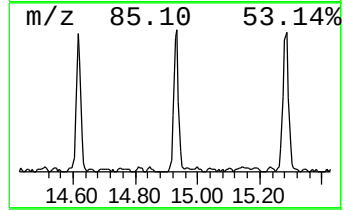
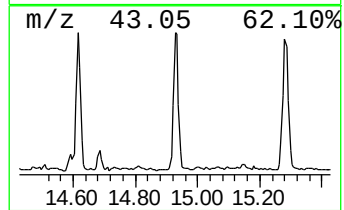
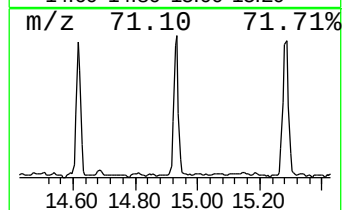
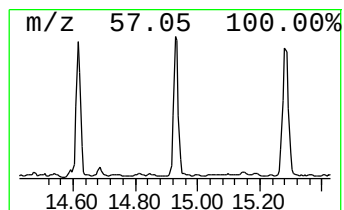
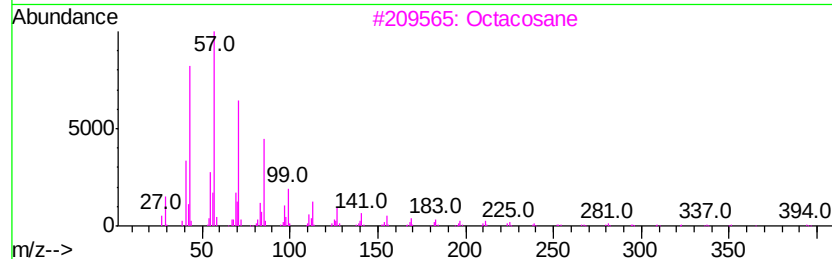
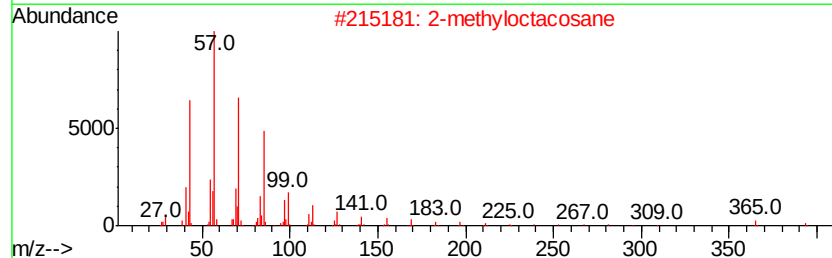
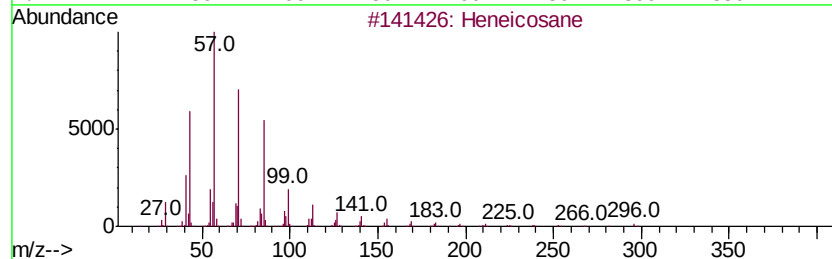
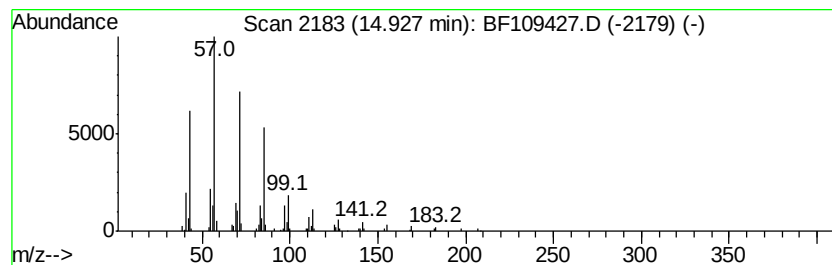
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	7.19 ng	185308	Perylene-d12	15.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	2-methyloctacosane		408	C29H60	1000376-72-8	91
3	Octacosane		394	C28H58	000630-02-4	91
4	Heptadecane		240	C17H36	000629-78-7	91
5	Hexacosane		366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
Data File : BF109427.D
Acq On : 28 Sep 2018 11:24
Operator : JU/SJ
Sample : J5133-07
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
092618-DBRI-F-D-B

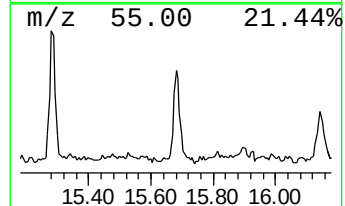
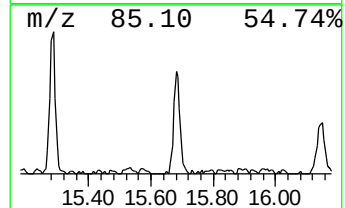
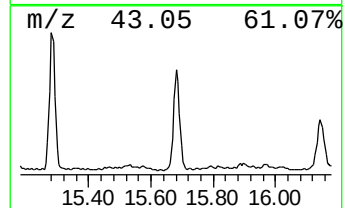
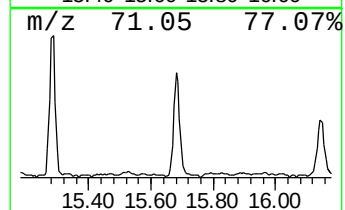
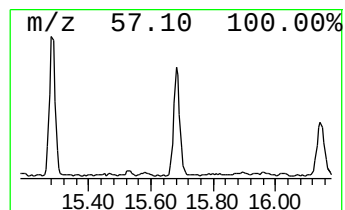
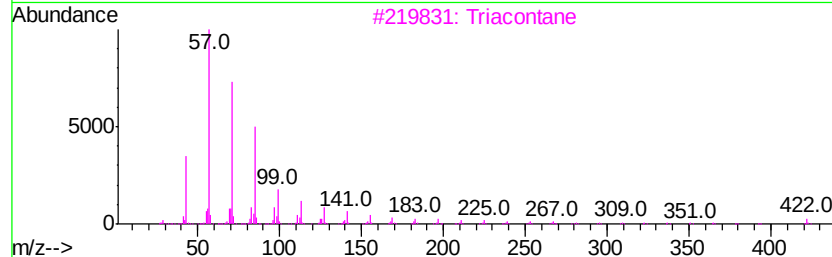
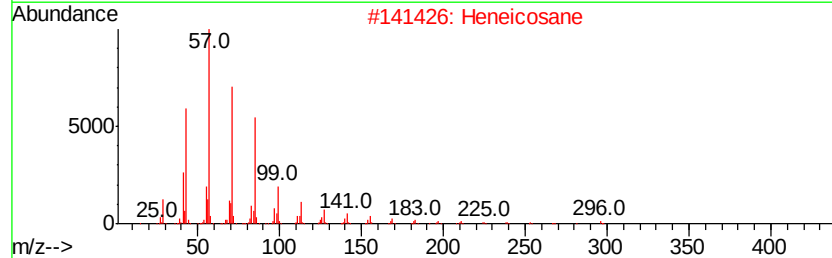
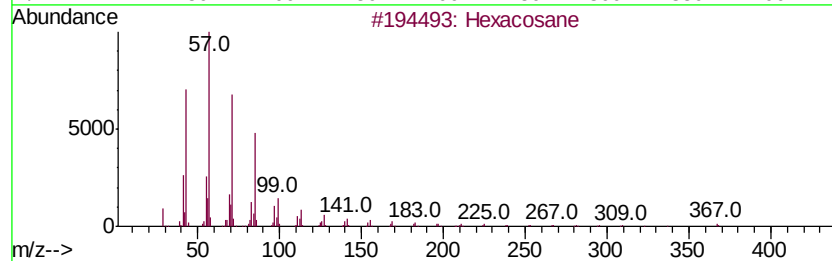
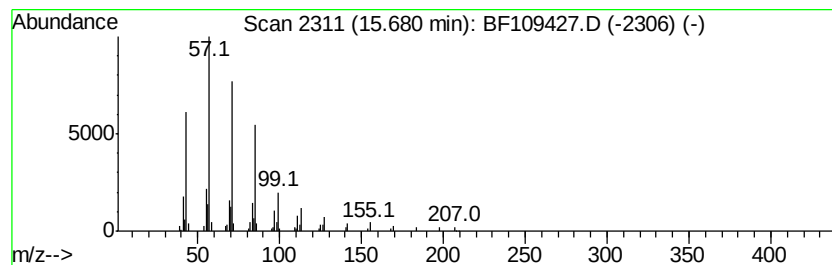
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.68	6.39 ng	164762	Perylene-d12	15.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	Triacontane		422	C30H62	000638-68-6	90
4	Octadecane, 1-iodo-		380	C18H37I	000629-93-6	87
5	Octacosane		394	C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
Data File : BF109427.D
Acq On : 28 Sep 2018 11:24
Operator : JU/SJ
Sample : J5133-07
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
092618-DBRI-F-D-B

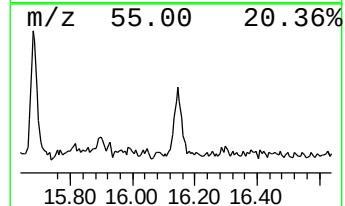
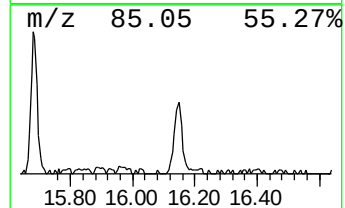
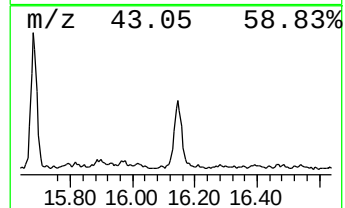
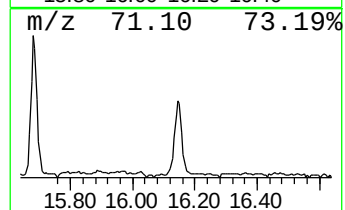
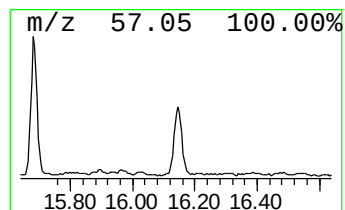
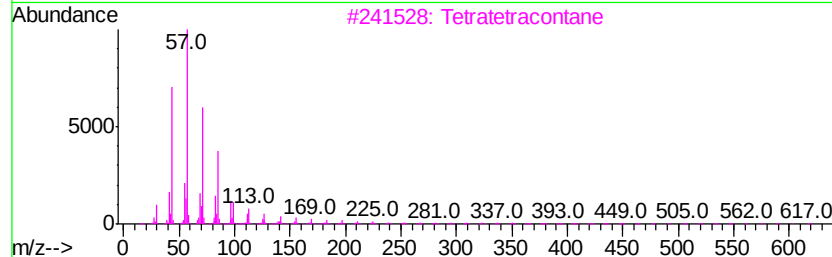
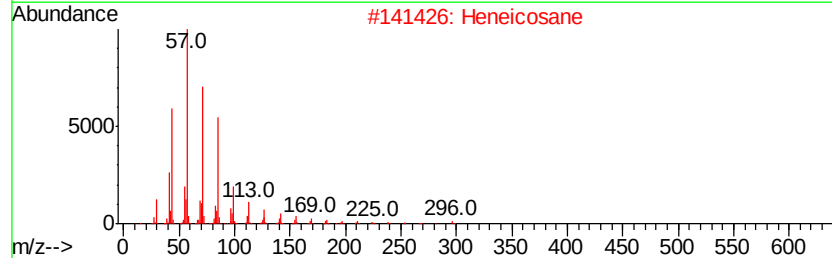
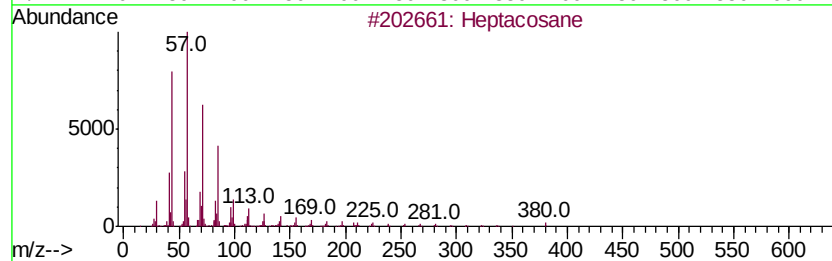
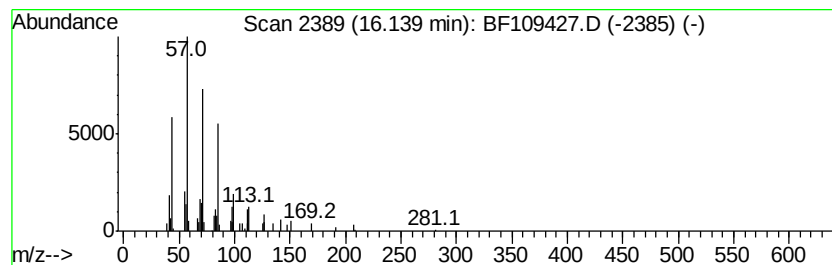
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.14	3.98 ng	102457	Perylene-d12	15.24

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Tetratetracontane	619	C44H90	007098-22-8	91
4			2-methyloctacosane	408	C29H60	1000376-72-8	91
5			Hentriacontane	437	C31H64	000630-04-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092718\
Data File : BF109427.D
Acq On : 28 Sep 2018 11:24
Operator : JU/SJ
Sample : J5133-07
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
092618-DBRI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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
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unknown6.47	6.47	51.1	ng	1494250	1	6.70	584431	20.0
unknown13.73	13.73	2.6	ng	86752	5	13.84	665572	20.0
Heptadecane, 9-oc...	14.32	3.0	ng	98543	5	13.84	665572	20.0
9-Octadecenamide,...	14.59	2.1	ng	53802	6	15.24	515343	20.0
Tetracosane	14.62	5.8	ng	150322	6	15.24	515343	20.0
Supraene	14.69	15.4	ng	396737	6	15.24	515343	20.0
Heneicosane	14.93	7.2	ng	185308	6	15.24	515343	20.0
Hexacosane	15.68	6.4	ng	164762	6	15.24	515343	20.0
Heptacosane	16.14	4.0	ng	102457	6	15.24	515343	20.0