

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102419\
 Data File : BF117512.D
 Acq On : 24 Oct 2019 16:13
 Operator : JU
 Sample : K5497-11
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 167-58-(0-1)

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-BF101819.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	5.357	552	556	582	rBV	774544	906544	88.52%	9.420%
2	6.381	727	730	748	rBV	934595	1008479	98.48%	10.479%
3	6.510	748	752	761	rVB	1037053	1024094	100.00%	10.641%
4	6.733	787	790	802	rBV	309190	277677	27.11%	2.885%
5	6.886	813	816	833	rBV	795595	717121	70.02%	7.452%
6	7.298	882	886	900	rBV	621834	595575	58.16%	6.189%
7	8.016	1004	1008	1025	rBV	364233	368633	36.00%	3.830%
8	9.086	1186	1190	1193	rBV	1212202	956754	93.42%	9.942%
9	9.480	1254	1257	1267	rBB	85976	76197	7.44%	0.792%
10	9.763	1301	1305	1320	rVB	528085	437986	42.77%	4.551%
11	10.557	1436	1440	1452	rBV	641355	610298	59.59%	6.342%
12	11.251	1554	1558	1561	rBV	411286	385038	37.60%	4.001%
13	11.780	1644	1648	1655	rBV	85377	91674	8.95%	0.953%
14	12.463	1761	1764	1775	rBV	38702	46922	4.58%	0.488%
15	12.557	1777	1780	1785	rBV2	31418	35615	3.48%	0.370%
16	12.692	1798	1803	1807	rBV	29952	31716	3.10%	0.330%
17	12.833	1822	1827	1830	rBV	755108	739316	72.19%	7.682%
18	13.298	1904	1906	1910	rBV	15707	16119	1.57%	0.167%
19	13.733	1976	1980	1993	rBV2	37811	66349	6.48%	0.689%
20	13.892	2003	2007	2015	rBV	297504	302462	29.53%	3.143%
21	14.045	2028	2033	2037	rBV	27883	29839	2.91%	0.310%
22	14.351	2082	2085	2089	rBV	45640	43876	4.28%	0.456%
23	14.651	2133	2136	2140	rVB	74810	66859	6.53%	0.695%
24	14.927	2180	2183	2186	rBV3	12084	18744	1.83%	0.195%
25	14.968	2186	2190	2194	rVB	90047	95853	9.36%	0.996%
26	15.215	2229	2232	2238	rBV3	11701	15880	1.55%	0.165%
27	15.327	2246	2251	2261	rVB2	297601	404254	39.47%	4.201%
28	15.733	2314	2320	2326	rBV	71532	111047	10.84%	1.154%
29	16.198	2393	2399	2408	rVB2	47029	80914	7.90%	0.841%
30	16.745	2488	2492	2500	rVB6	20211	41507	4.05%	0.431%
31	17.392	2596	2602	2609	rBV9	9367	20478	2.00%	0.213%

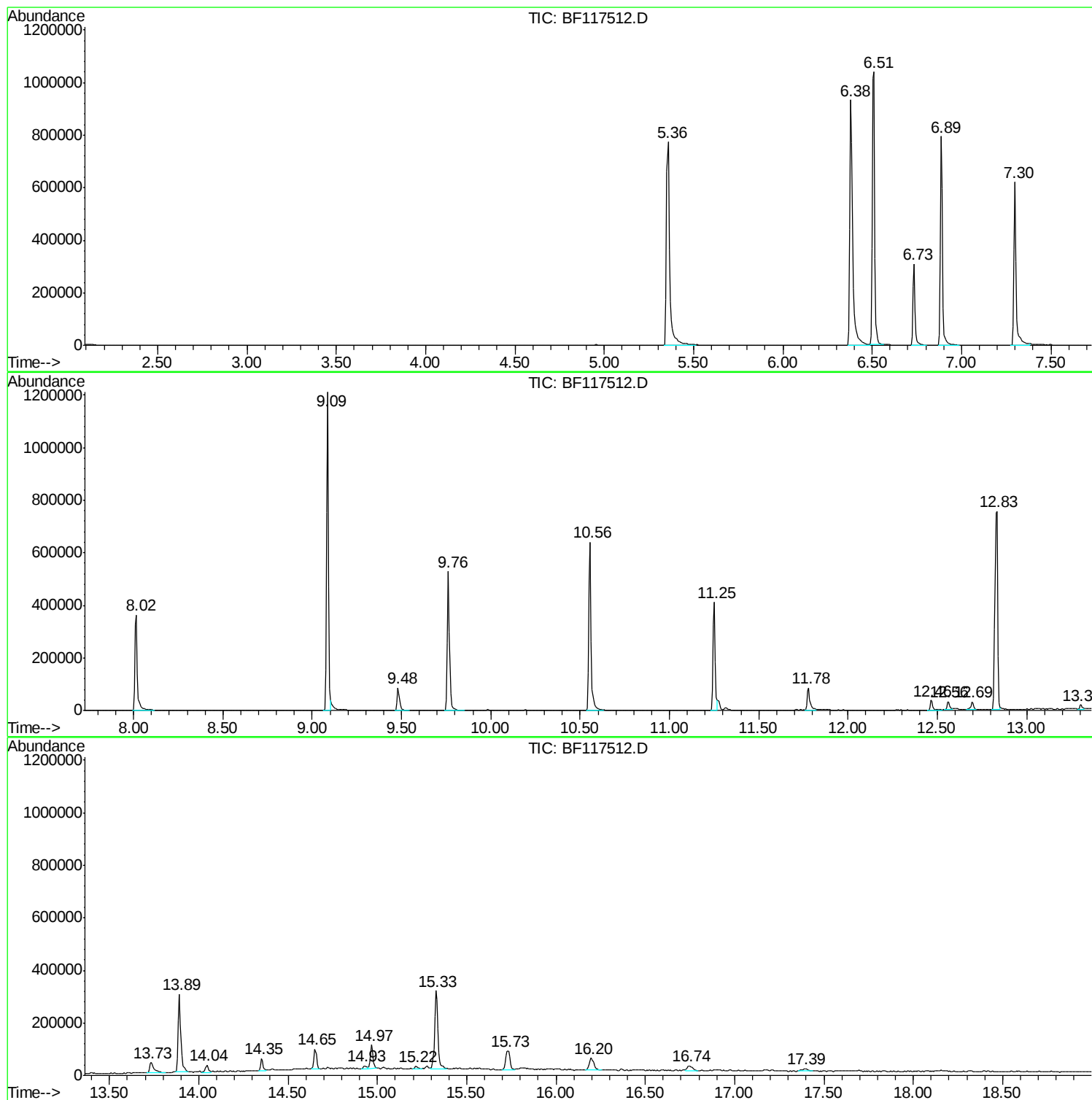
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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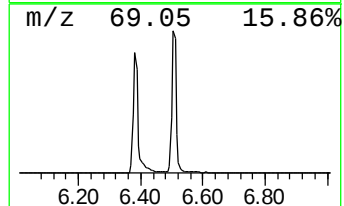
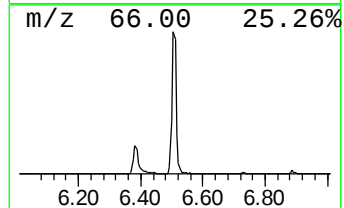
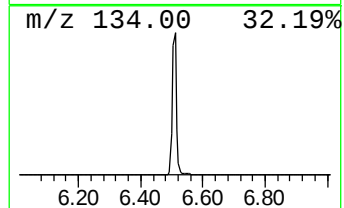
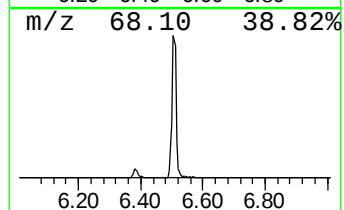
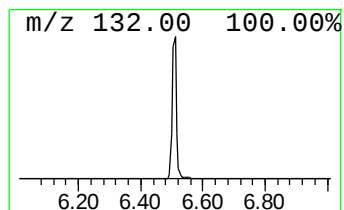
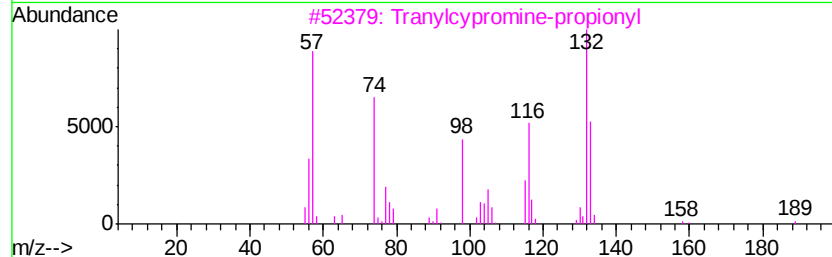
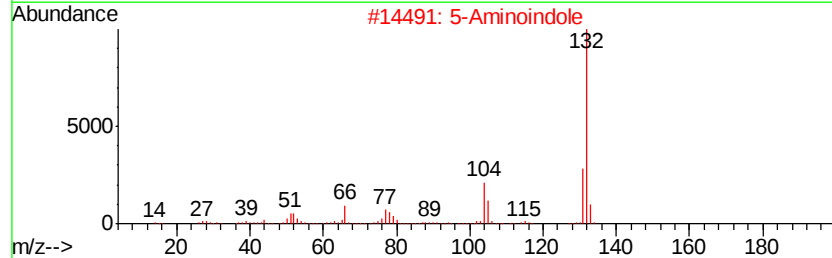
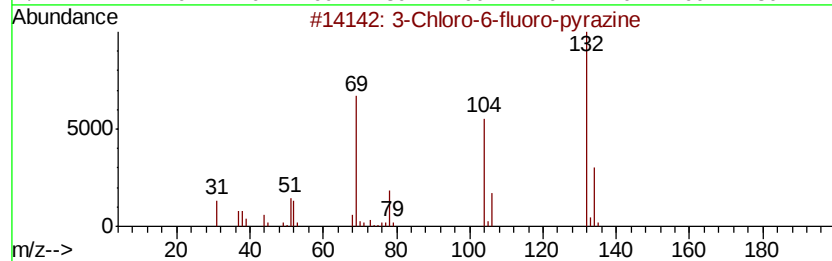
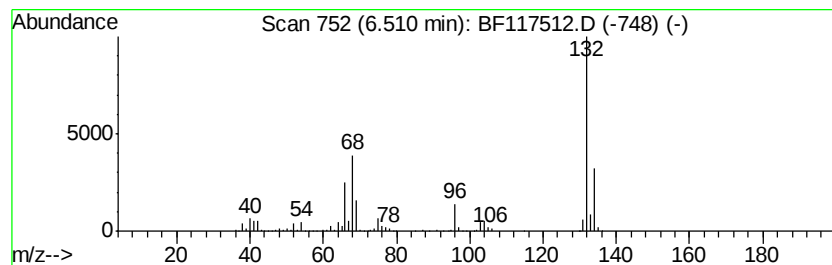
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	73.76 ng	1024090	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Aminoindole	132	C8H8N2	005192-03-0	12	
3	Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	12	
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10	
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9	



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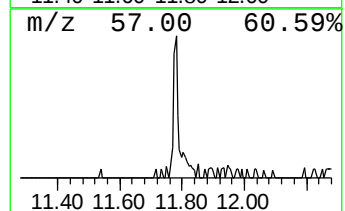
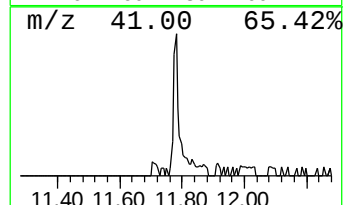
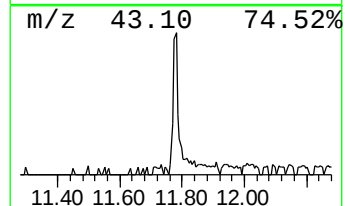
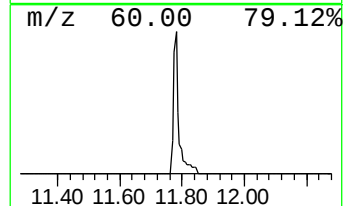
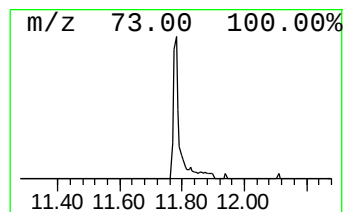
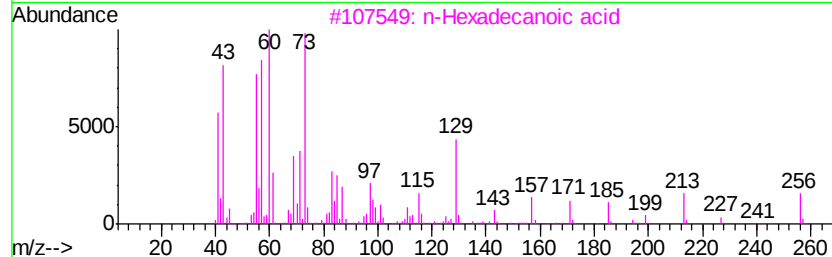
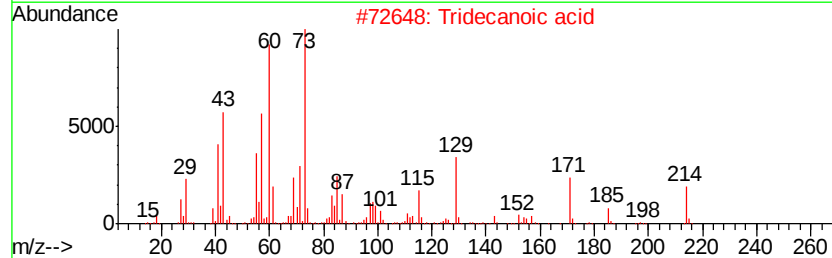
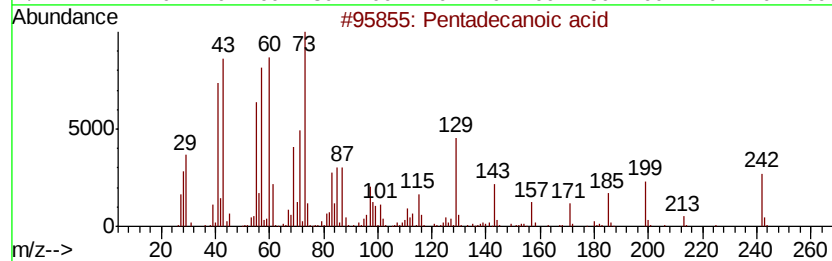
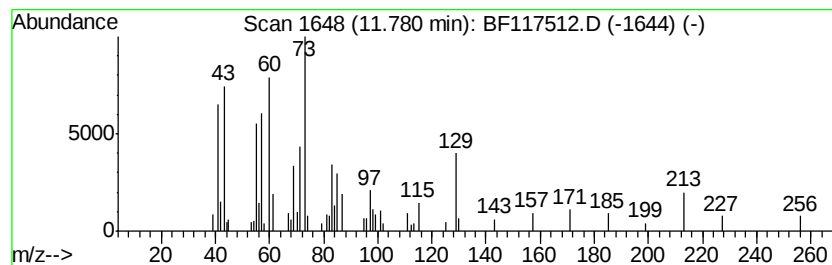
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Peak Number 3 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	4.76 ng	91674	Phenanthrene-d10	11.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
2		Tridecanoic acid	214	C13H26O2	000638-53-9	64
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
4		.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	18
5		Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	14



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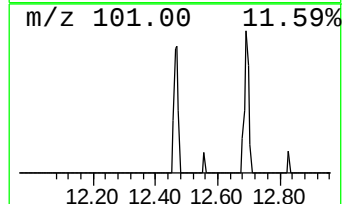
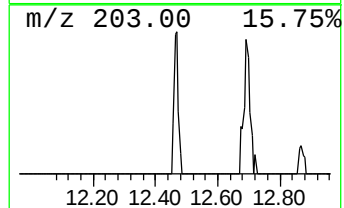
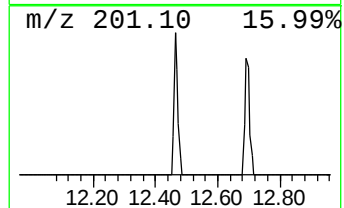
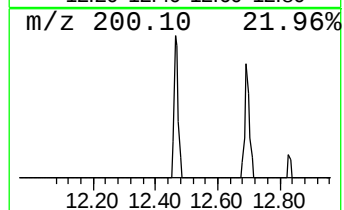
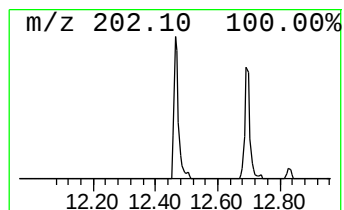
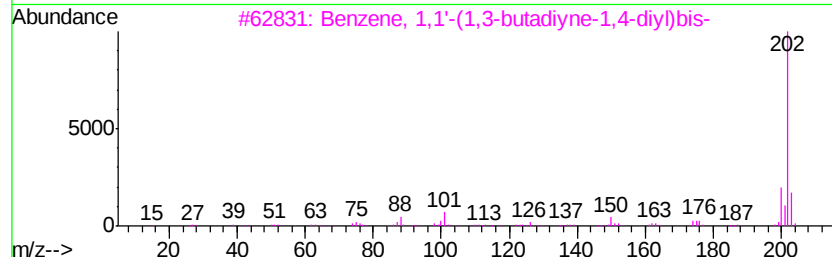
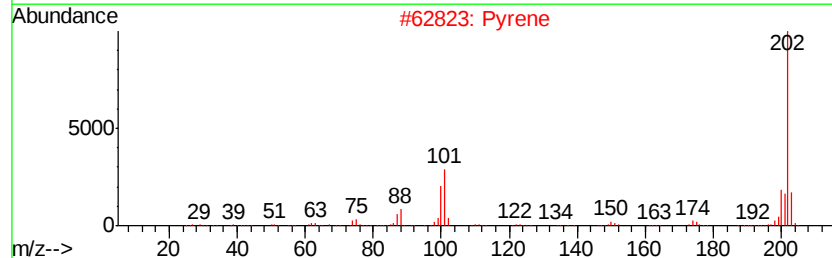
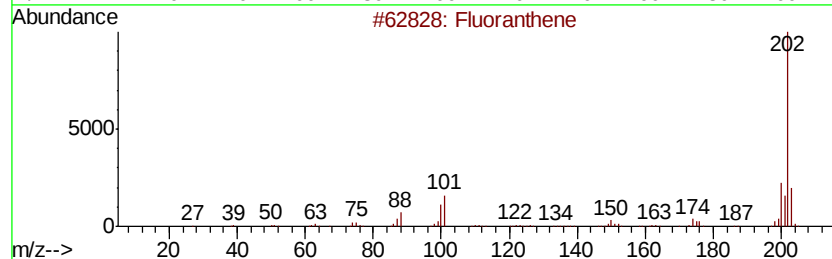
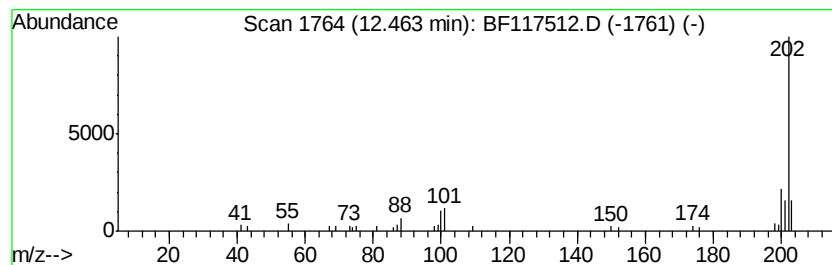
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	2.44 ng	46922	Phenanthrene-d10	11.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Fluoranthene	202	C16H10	000206-44-0	95
2		Pyrene	202	C16H10	000129-00-0	83
3		Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	58
4		4-Methoxy-naphthalene-1-carboxyl...	202	C12H10O3	1000317-85-4	38
5		3-(4-Pyridinylmethyl)-3-azabicyc...	202	C11H10N2O2	1000332-54-9	9



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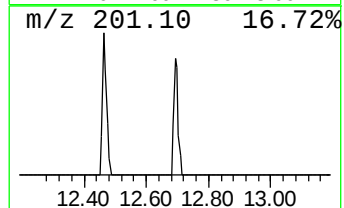
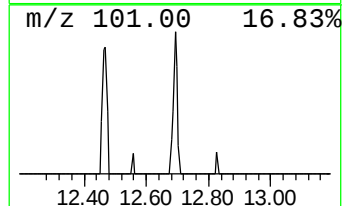
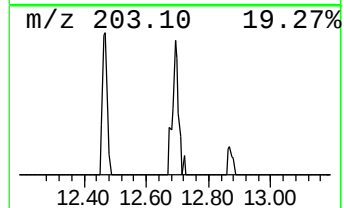
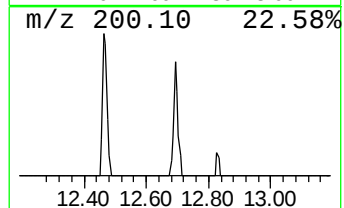
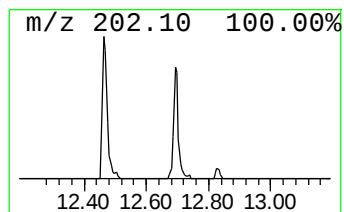
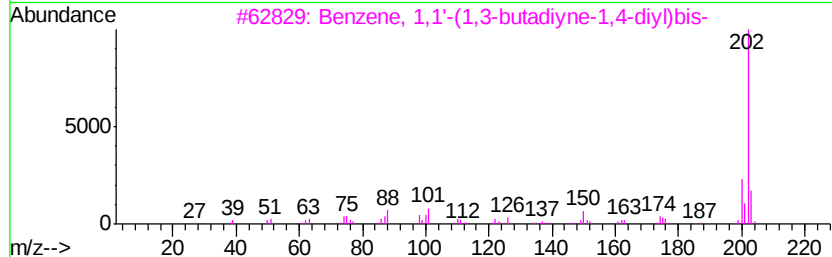
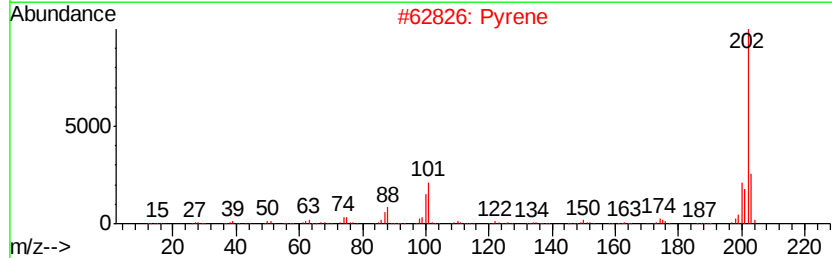
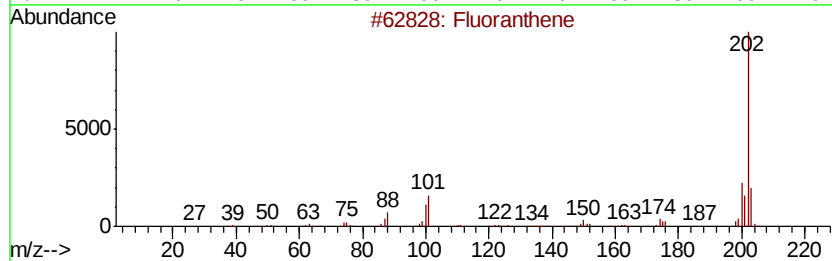
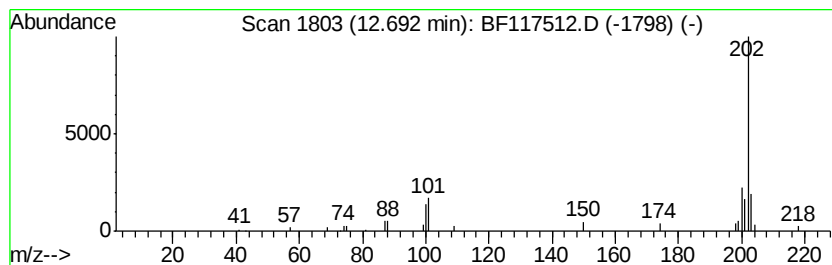
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Peak Number 5 unknown12.69 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.69	2.10 ng	31716	Chrysene-d12	13.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Fluoranthene	202	C16H10	000206-44-0	91
2		Pyrene	202	C16H10	000129-00-0	87
3		Benzene, 1,1'-(1,3-butadiene-1,4...	202	C16H10	000886-66-8	64
4		5-(4-Methylphenyl)furan-2-carbox...	202	C12H10O3	1000305-27-5	40
5		4-Methoxy-naphthalene-1-carboxyl...	202	C12H10O3	1000317-85-4	37



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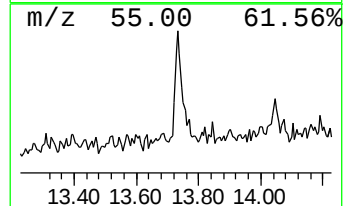
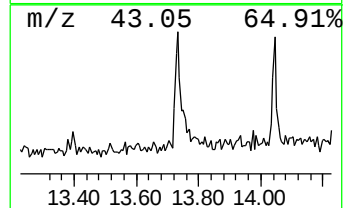
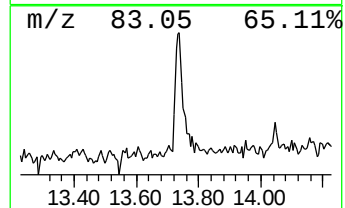
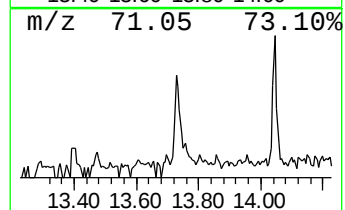
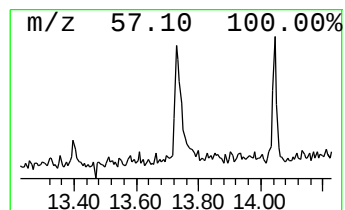
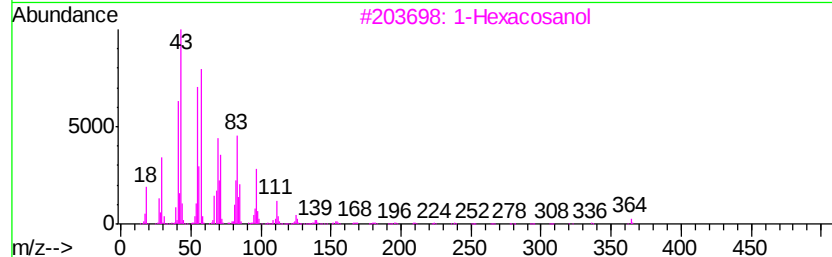
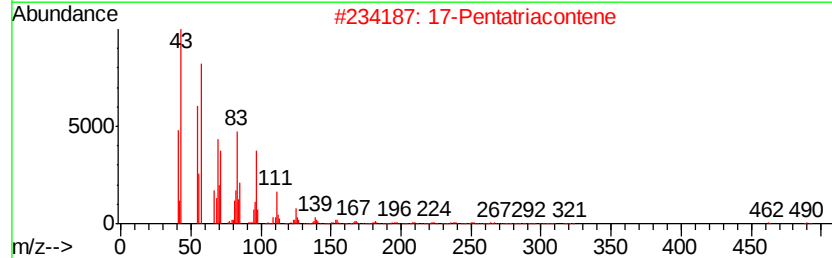
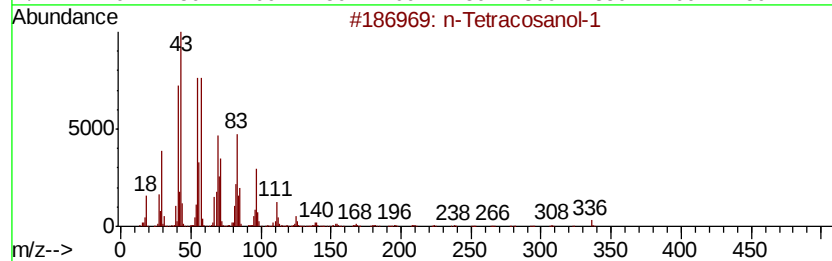
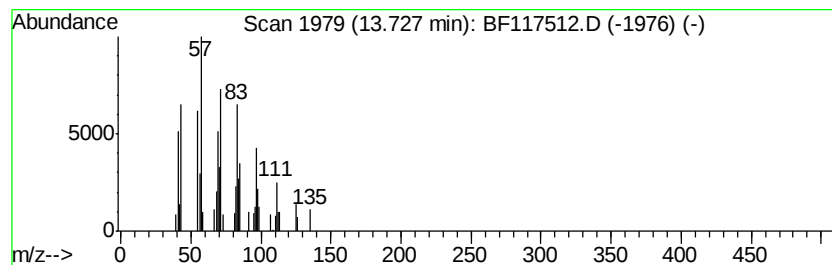
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Peak Number 6 n-Tetracosanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	4.39 ng	66349	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
2		17-Pentatriacontene	491	C35H70	006971-40-0	90
3		1-Hexacosanol	382	C26H54O	000506-52-5	90
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
5		11-Tricosene	322	C23H46	052078-56-5	87



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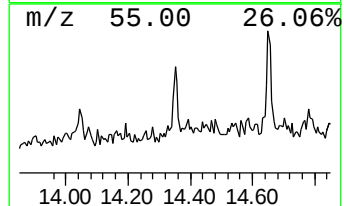
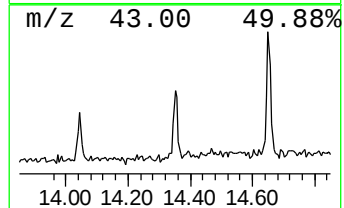
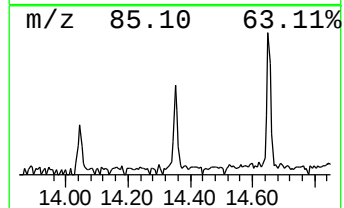
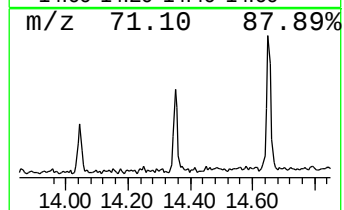
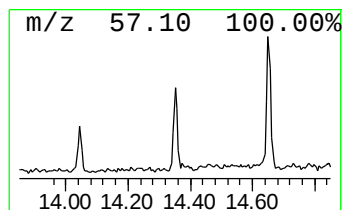
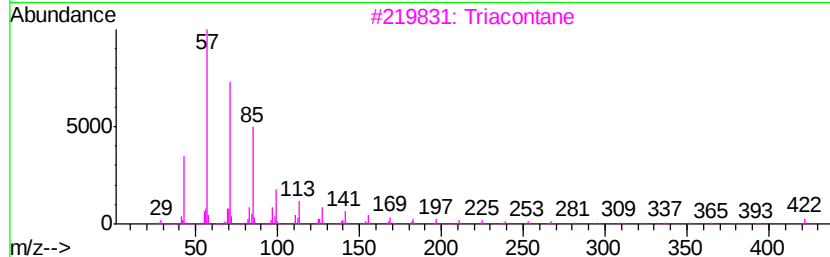
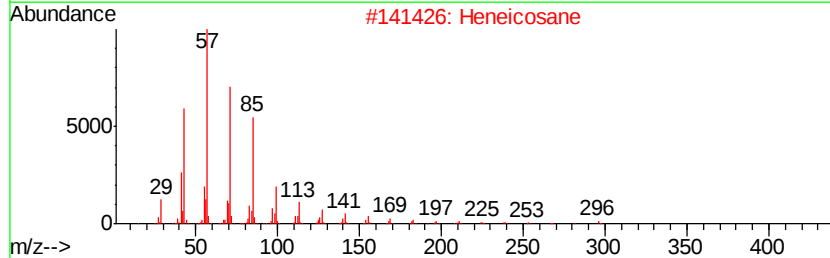
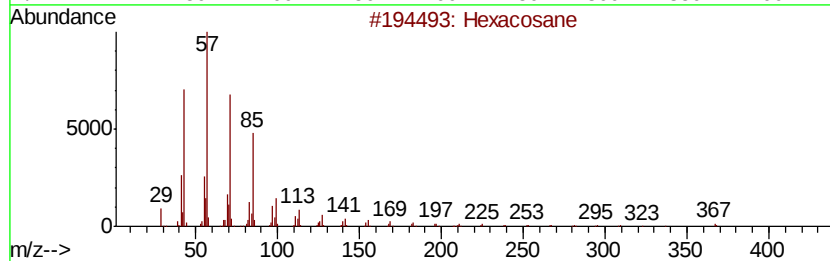
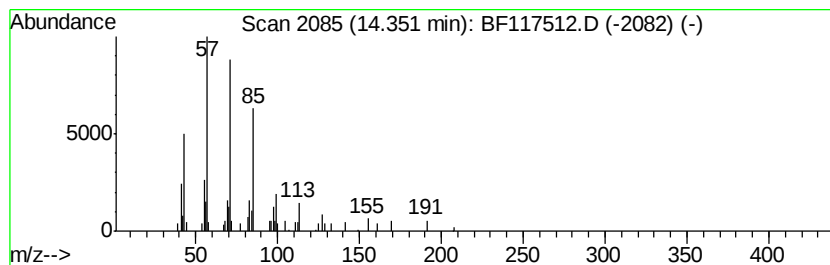
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	2.90 ng	43876	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Triacontane	422	C30H62	000638-68-6	90
4		Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
5		Pentacosane	352	C25H52	000629-99-2	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102419\
Data File : BF117512.D
Acq On : 24 Oct 2019 16:13
Operator : JU
Sample : K5497-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
167-58-(0-1)

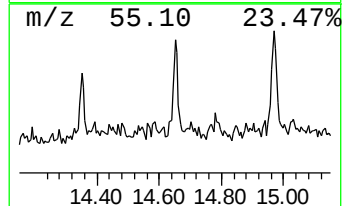
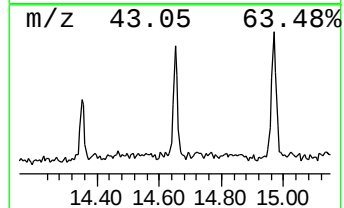
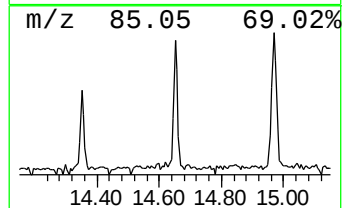
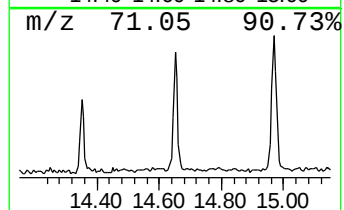
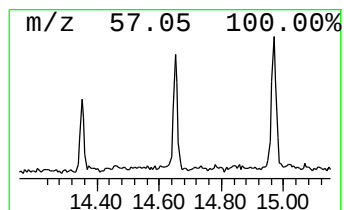
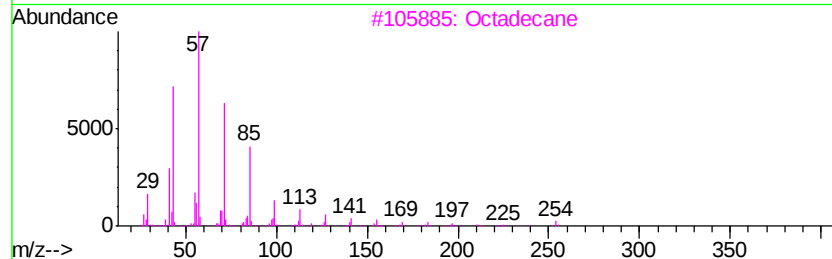
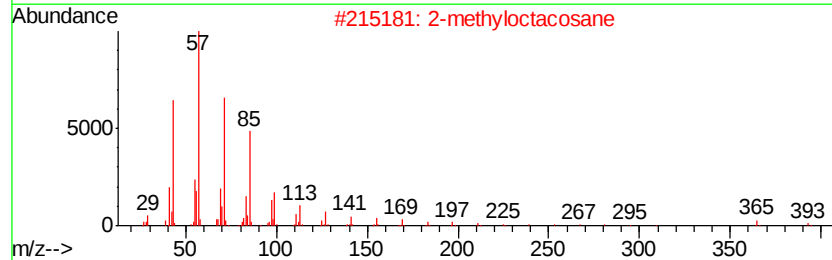
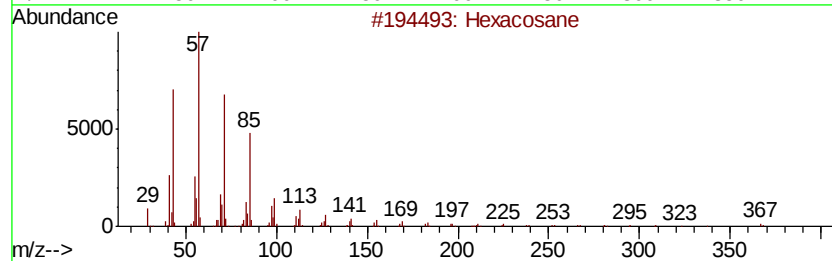
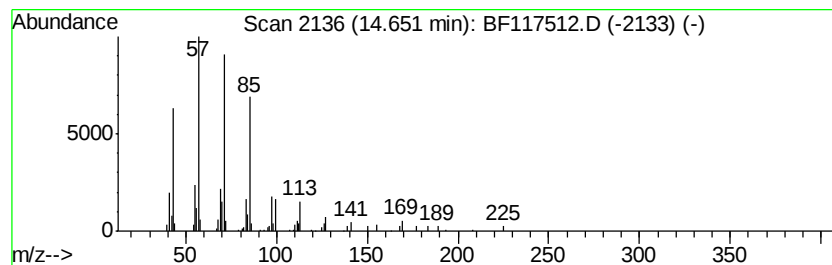
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	3.31 ng	66859	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	90
3		Octadecane	254	C18H38	000593-45-3	86
4		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
5		Heptacosane	380	C27H56	000593-49-7	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102419\
Data File : BF117512.D
Acq On : 24 Oct 2019 16:13
Operator : JU
Sample : K5497-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
167-58-(0-1)

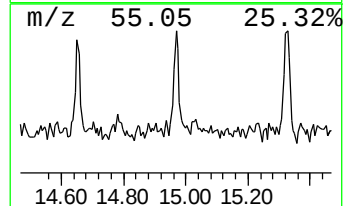
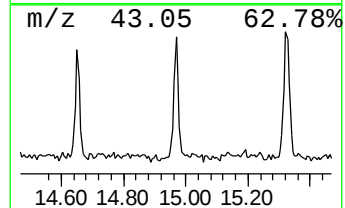
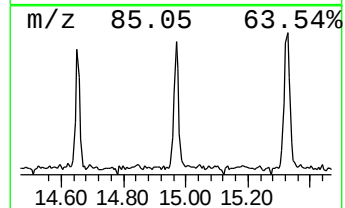
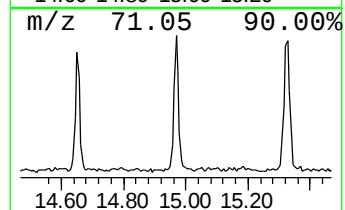
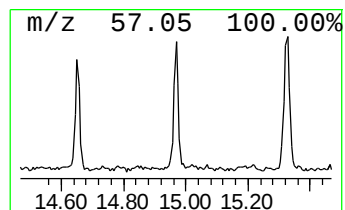
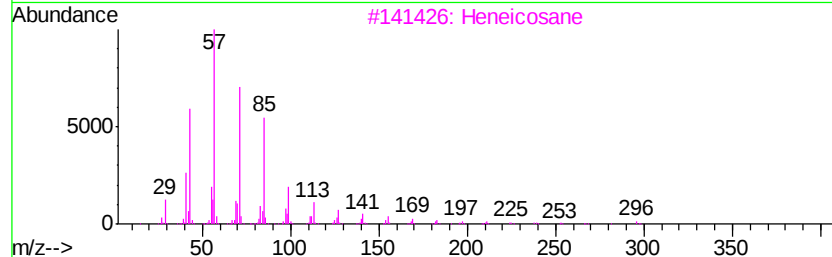
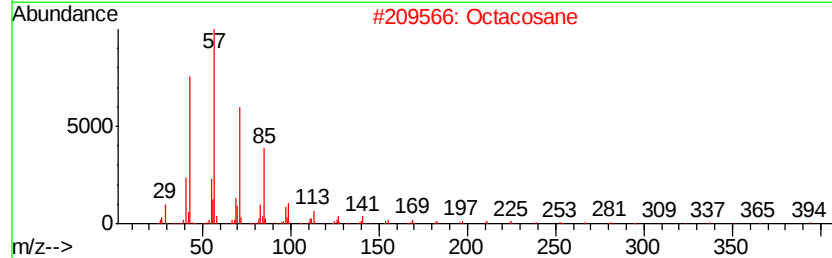
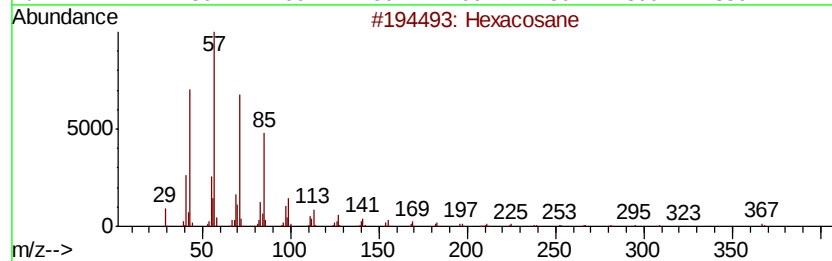
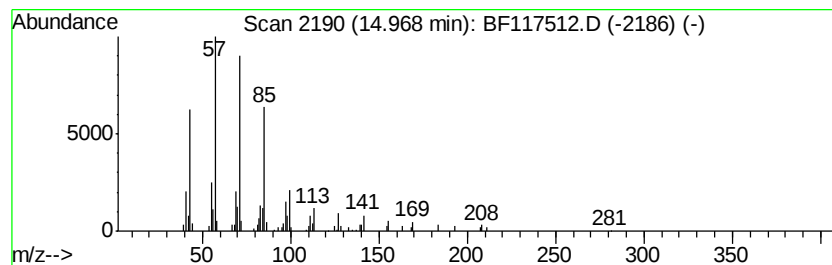
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	4.74 ng	95853	Perylene-d12	15.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	Octacosane		394	C28H58	000630-02-4	91
3	Heneicosane		296	C21H44	000629-94-7	91
4	triacontane		422	C30H62	000638-68-6	91
5	2-methyloctacosane		408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102419\
Data File : BF117512.D
Acq On : 24 Oct 2019 16:13
Operator : JU
Sample : K5497-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
167-58-(0-1)

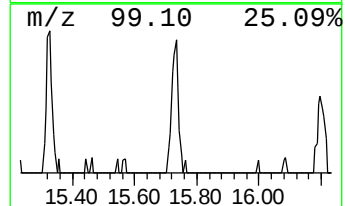
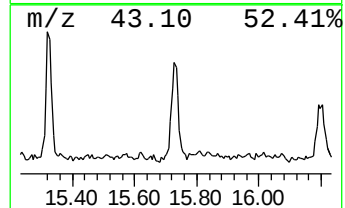
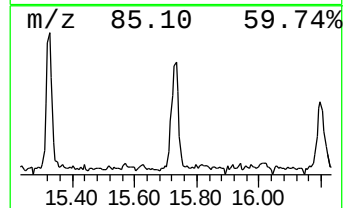
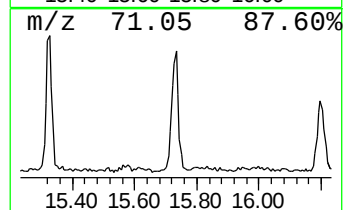
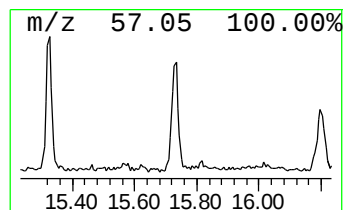
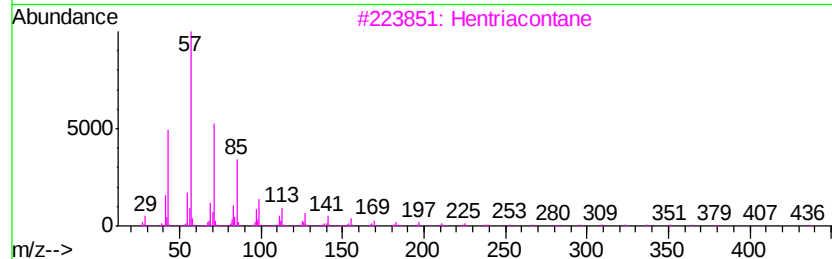
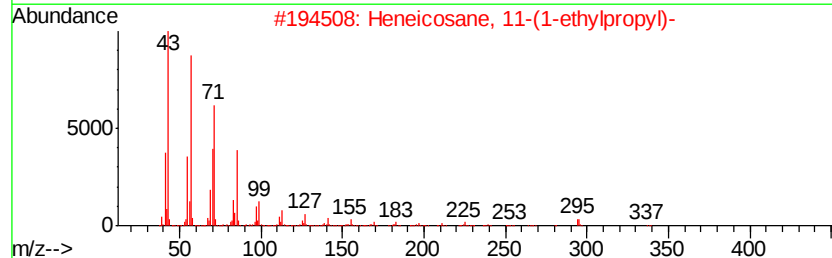
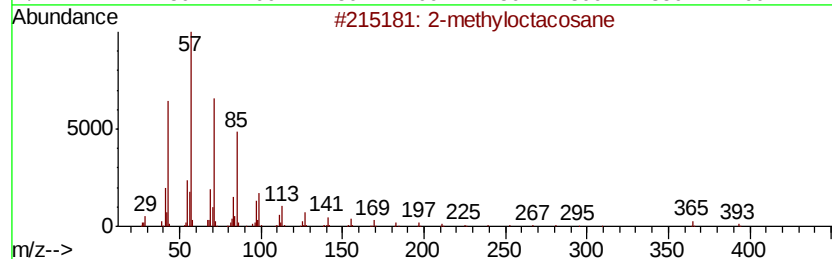
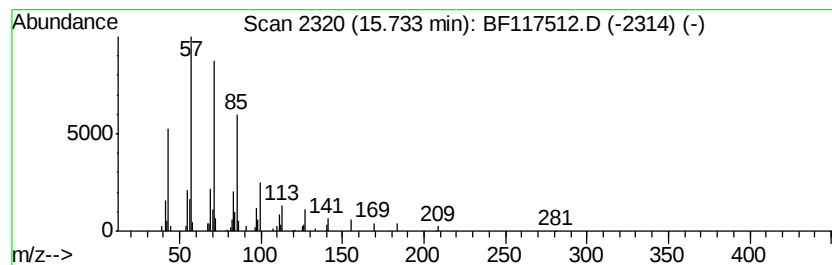
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-methyloctacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	5.49 ng	111047	Perylene-d12	15.33

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-methyloctacosane	408	C29H60	1000376-72-8	91
2			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
3			Hentriacontane	437	C31H64	000630-04-6	87
4			Hexacosane	366	C26H54	000630-01-3	87
5			Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102419\
Data File : BF117512.D
Acq On : 24 Oct 2019 16:13
Operator : JU
Sample : K5497-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
167-58-(0-1)

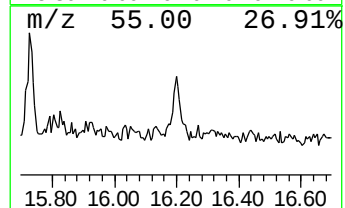
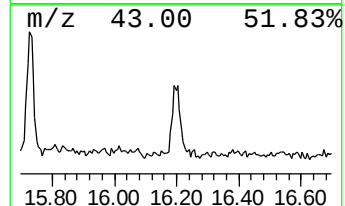
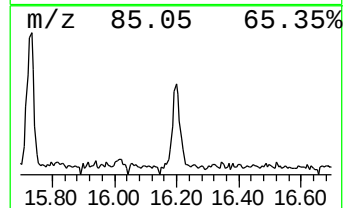
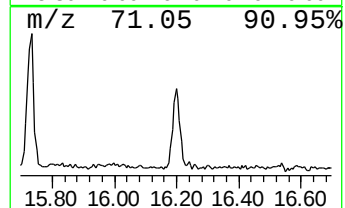
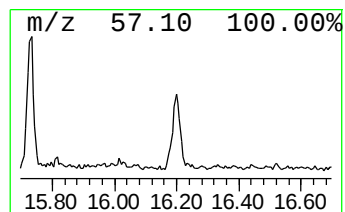
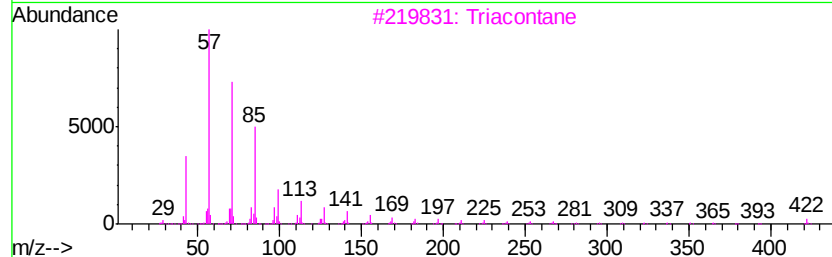
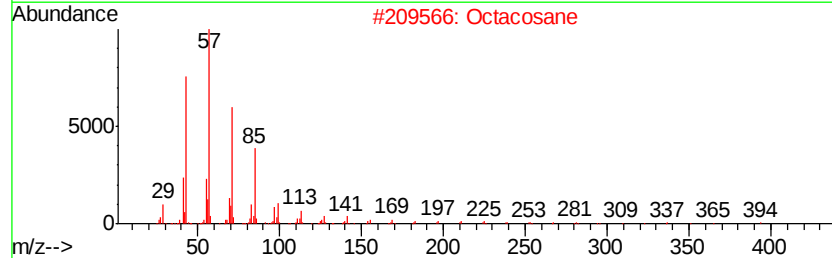
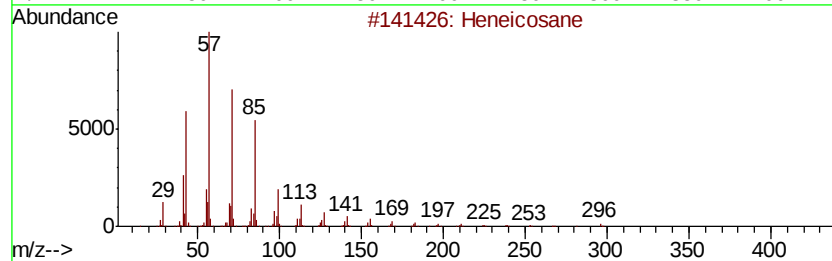
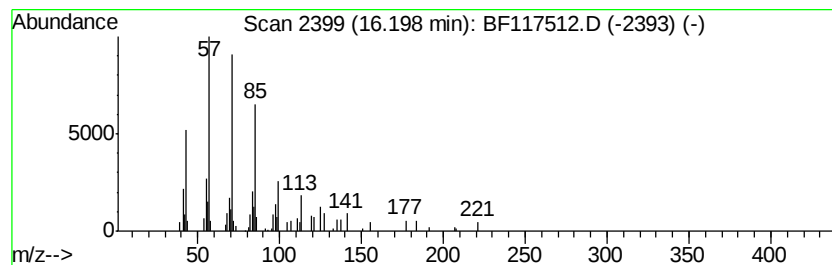
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Triacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.20	4.00 ng	80914	Perylene-d12	15.33

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	90
2			Octacosane	394	C28H58	000630-02-4	90
3			Triacontane	422	C30H62	000638-68-6	80
4			Hexacosane	366	C26H54	000630-01-3	80
5			Heptadecane	240	C17H36	000629-78-7	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102419\
Data File : BF117512.D
Acq On : 24 Oct 2019 16:13
Operator : JU
Sample : K5497-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
167-58-(0-1)

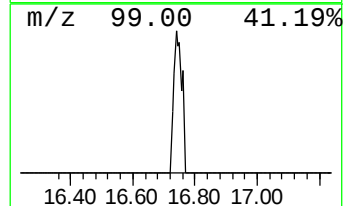
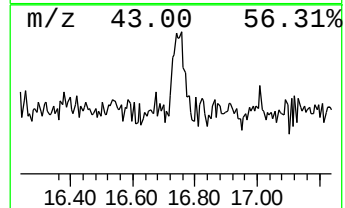
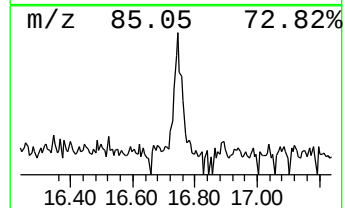
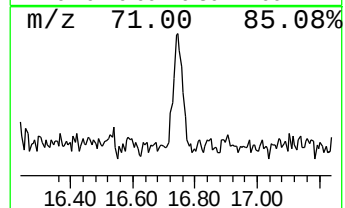
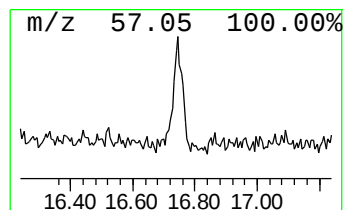
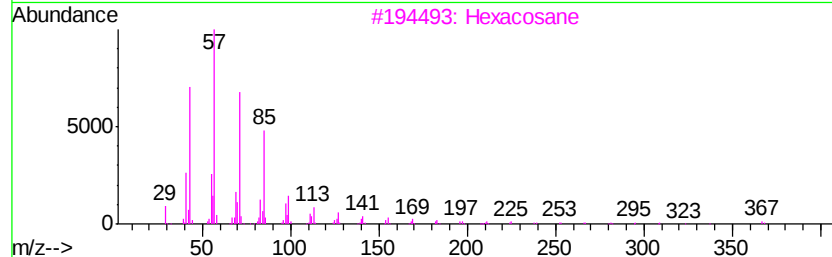
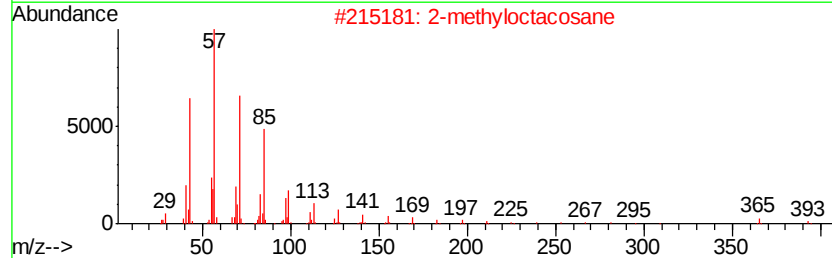
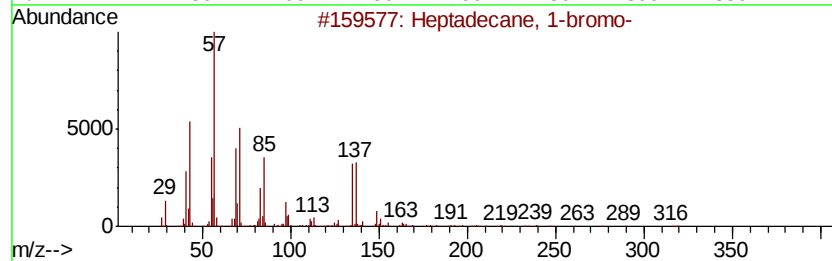
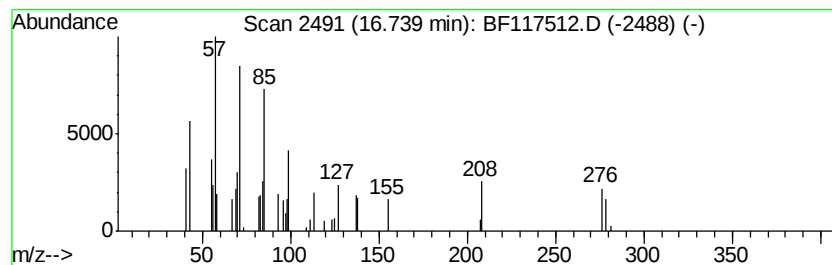
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heptadecane, 1-bromo- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.74	2.05 ng	41507	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 1-bromo-	318	C17H35Br	003508-00-7	50
2		2-methyloctacosane	408	C29H60	1000376-72-8	47
3		Hexacosane	366	C26H54	000630-01-3	47
4		Pentadecane	212	C15H32	000629-62-9	43
5		Nonadecane	268	C19H40	000629-92-5	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102419\
Data File : BF117512.D
Acq On : 24 Oct 2019 16:13
Operator : JU
Sample : K5497-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
167-58-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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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Pentadecanoic acid	11.78	4.8	ng	91674	4	11.25	385038	20.0
Benzene, 1,1'-(1,...	12.46	2.4	ng	46922	4	11.25	385038	20.0
unknown12.69	12.69	2.1	ng	31716	5	13.89	302462	20.0
n-Tetracosanol-1	13.73	4.4	ng	66349	5	13.89	302462	20.0
Heneicosane	14.35	2.9	ng	43876	5	13.89	302462	20.0
Hexacosane	14.65	3.3	ng	66859	6	15.33	404254	20.0
Octacosane	14.97	4.7	ng	95853	6	15.33	404254	20.0
2-methyloctacosane	15.73	5.5	ng	111047	6	15.33	404254	20.0
triacontane	16.20	4.0	ng	80914	6	15.33	404254	20.0
Heptadecane, 1-br...	16.74	2.0	ng	41507	6	15.33	404254	20.0