

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082118\
 Data File : BF108328.D
 Acq On : 21 Aug 2018 10:23
 Operator : JU/SJ
 Sample : J4500-16
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-7

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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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	3.219	145	150	155	rVB	71039	105214	1.42%	0.198%
2	5.278	495	500	512	rVB	638790	927935	12.51%	1.742%
3	5.654	558	564	567	rBV	4613529	4719970	63.61%	8.861%
4	6.637	725	731	734	rBV	4015696	4385714	59.10%	8.233%
5	6.784	750	756	759	rBV	5266381	5344247	72.02%	10.033%
6	7.007	790	794	797	rBV	1331583	1099283	14.81%	2.064%
7	7.166	816	821	824	rBV	4420508	4176734	56.29%	7.841%
8	7.572	884	890	893	rBV	3355953	3714203	50.05%	6.973%
9	8.289	1007	1012	1015	rBV	1423347	1397189	18.83%	2.623%
10	9.366	1188	1195	1198	rBV	6036813	6514366	87.79%	12.230%
11	10.048	1305	1311	1315	rBV	1642375	1624294	21.89%	3.049%
12	10.848	1440	1447	1450	rBV	4366363	4521591	60.94%	8.489%
13	11.548	1560	1566	1569	rBV	2019895	1778056	23.96%	3.338%
14	12.260	1683	1687	1695	rBV	64946	79690	1.07%	0.150%
15	12.930	1797	1801	1805	rVB	597514	473527	6.38%	0.889%
16	13.007	1811	1814	1819	rVB	135667	107537	1.45%	0.202%
17	13.142	1829	1837	1840	rBV	6629858	7420246	100.00%	13.930%
18	13.636	1918	1921	1925	rBV	469847	364750	4.92%	0.685%
19	13.924	1962	1970	1974	rBV4	44514	120251	1.62%	0.226%
20	14.013	1982	1985	1990	rVB	110986	101372	1.37%	0.190%
21	14.201	2013	2017	2021	rVB	1755921	1564972	21.09%	2.938%
22	14.330	2035	2039	2043	rVB	139463	136160	1.83%	0.256%
23	14.636	2087	2091	2096	rVB	169813	181812	2.45%	0.341%
24	14.960	2142	2146	2153	rBV	169727	197371	2.66%	0.371%
25	15.324	2204	2208	2215	rVB	200097	235475	3.17%	0.442%
26	15.759	2274	2282	2289	rVB2	771383	1335190	17.99%	2.507%
27	16.212	2354	2359	2366	rVB	192590	313991	4.23%	0.589%
28	16.771	2448	2454	2460	rVB	117224	231345	3.12%	0.434%
29	17.424	2561	2565	2575	rVB3	46372	94361	1.27%	0.177%

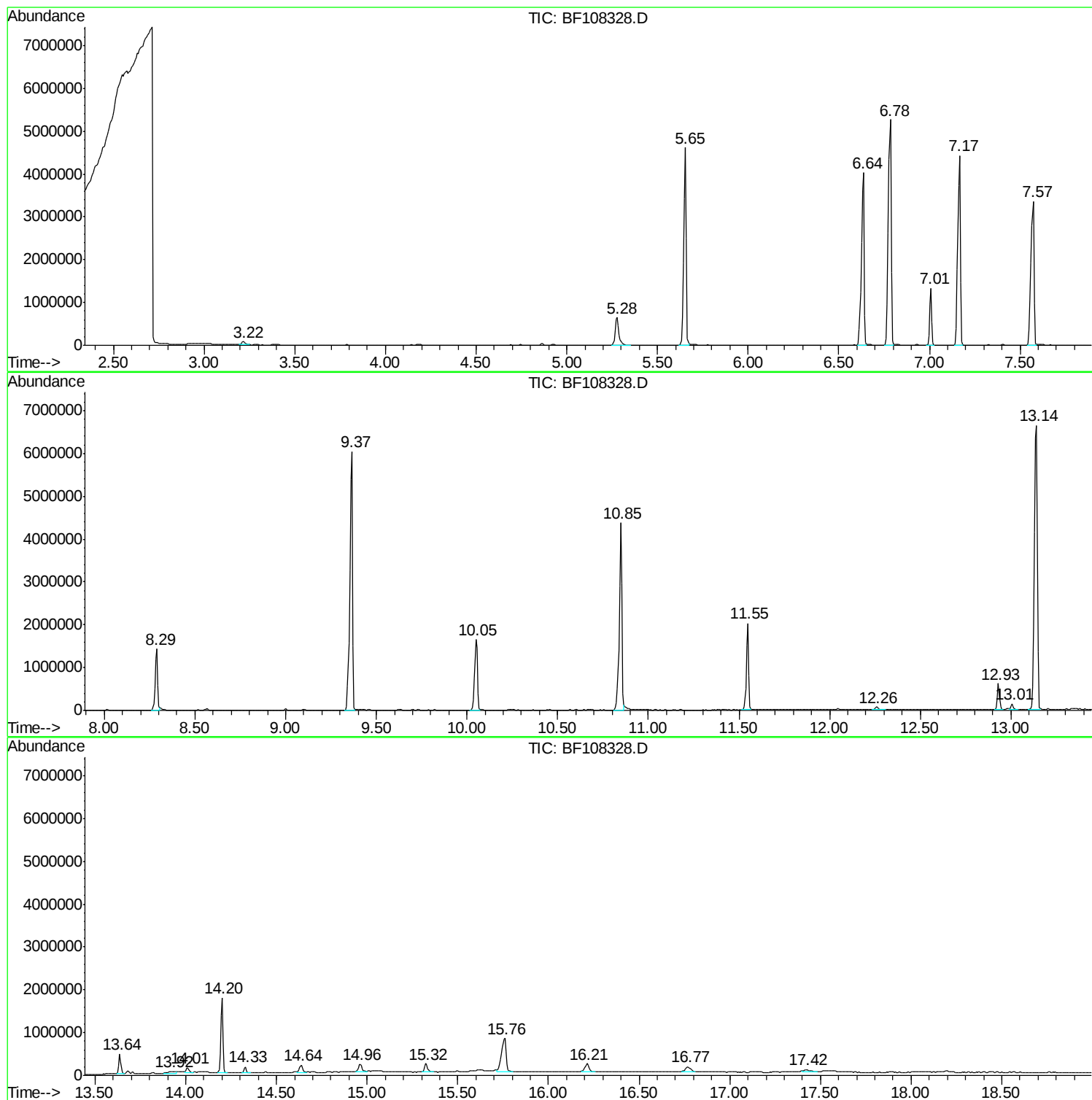
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ClientSampled :
TP-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.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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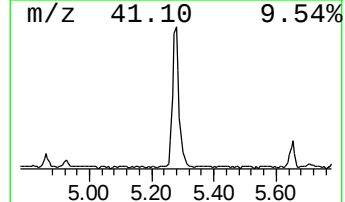
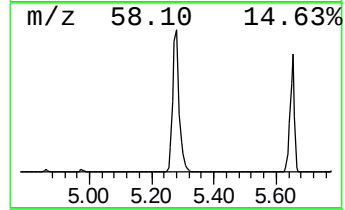
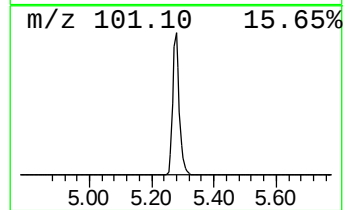
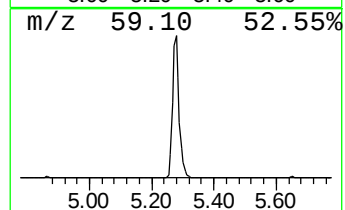
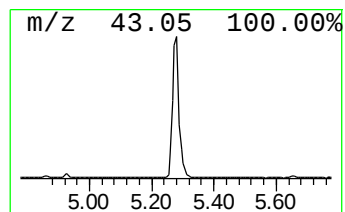
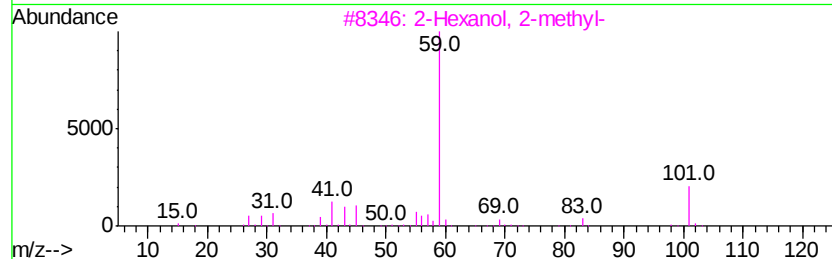
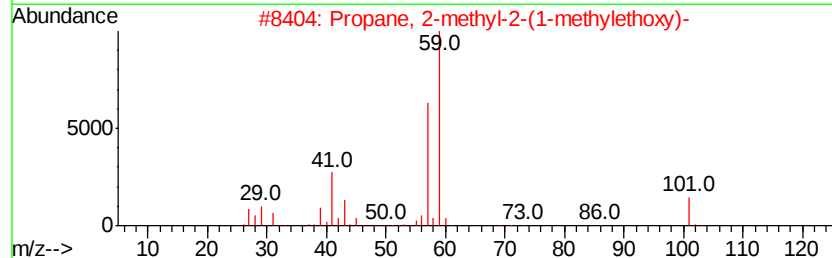
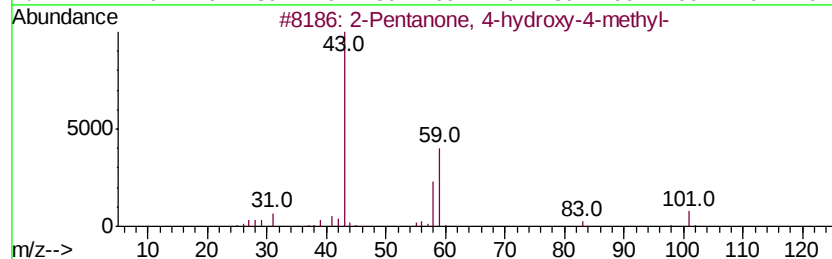
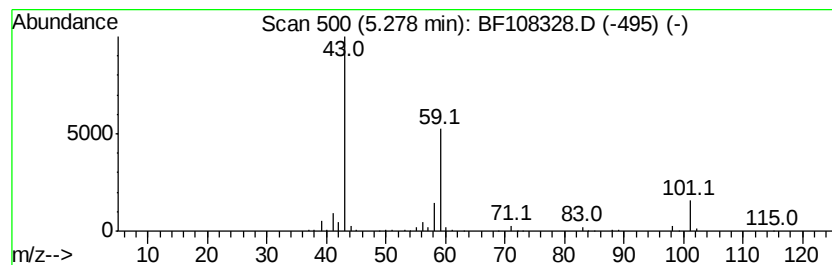
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.28	16.88 ng	927935	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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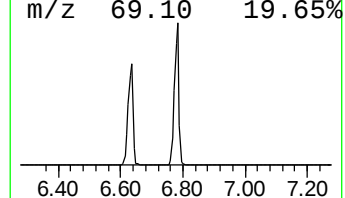
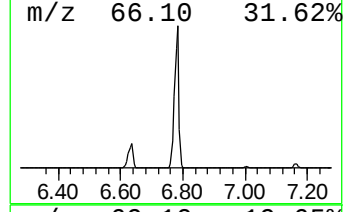
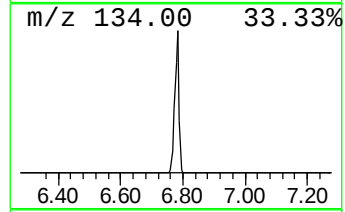
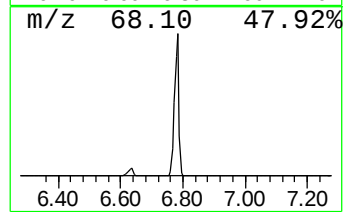
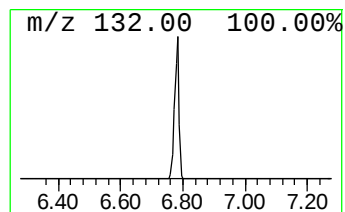
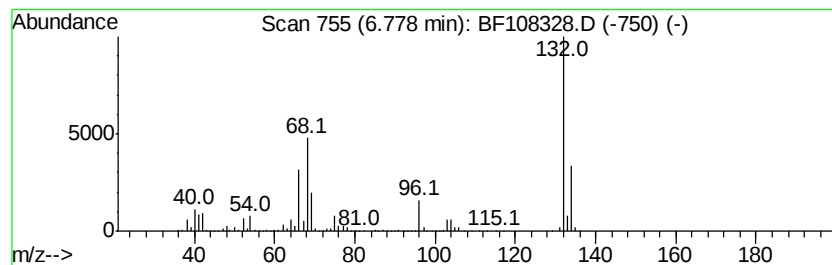
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	97.23 ng	5344250	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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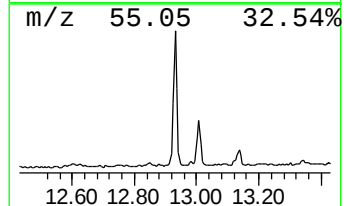
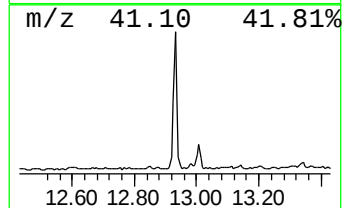
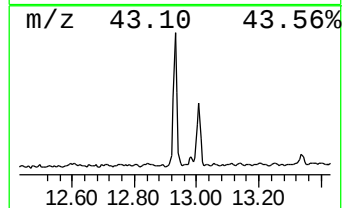
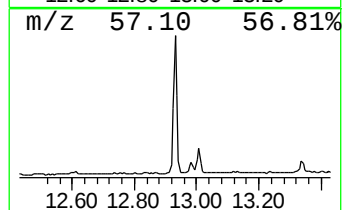
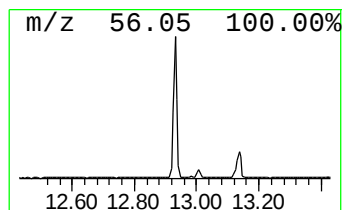
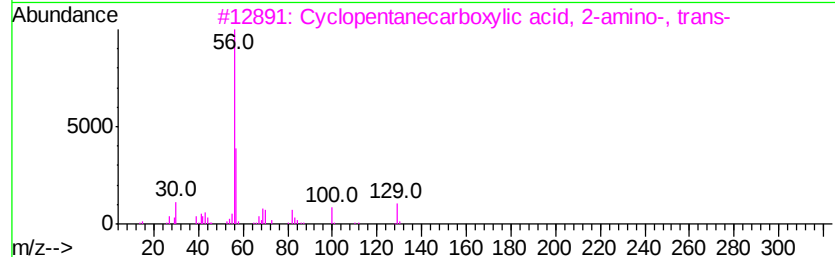
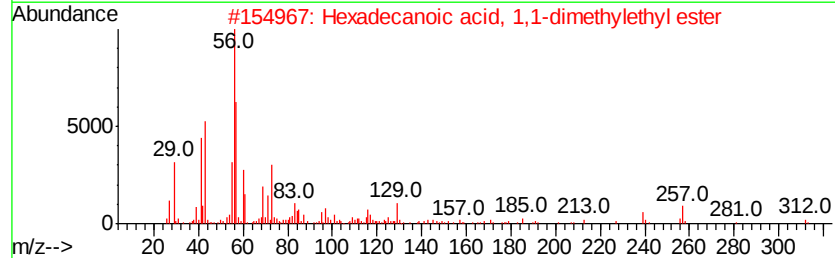
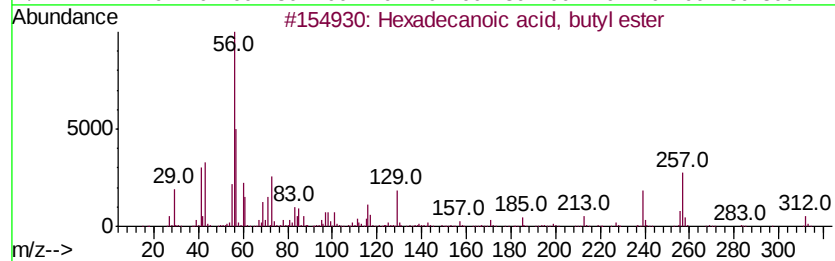
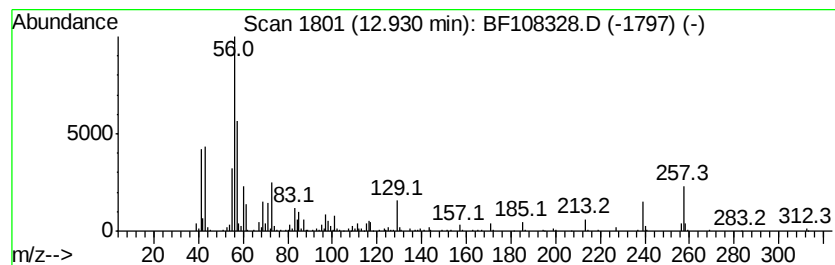
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.93	6.05 ng	473527	Chrysene-d12	14.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	60
3		Cyclopentanecarboxylic acid, 2-am...	129	C6H11NO2	040482-05-1	38
4		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	38
5		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	32



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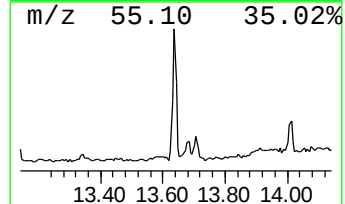
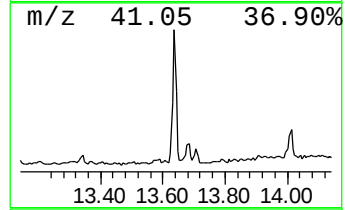
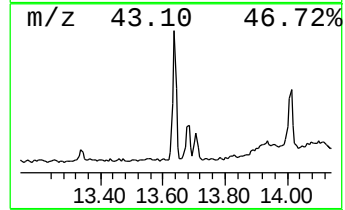
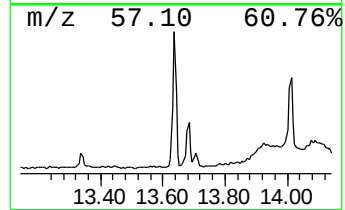
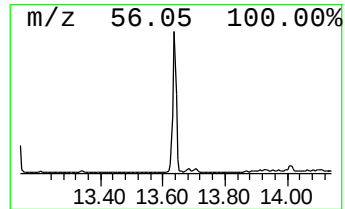
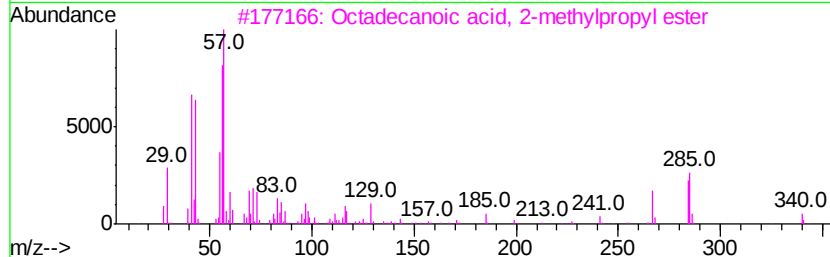
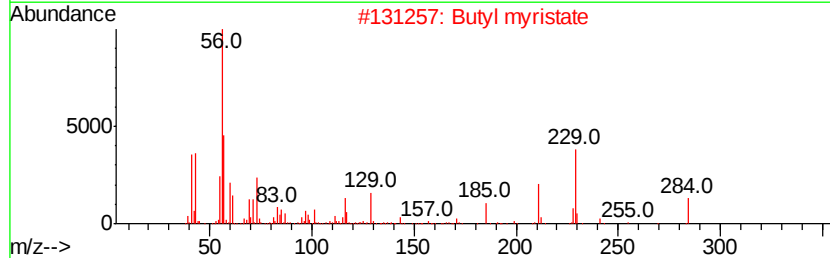
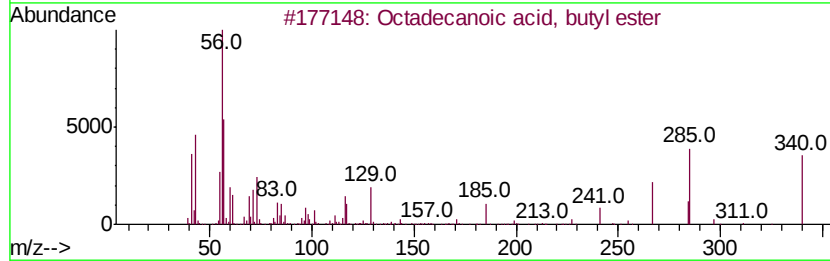
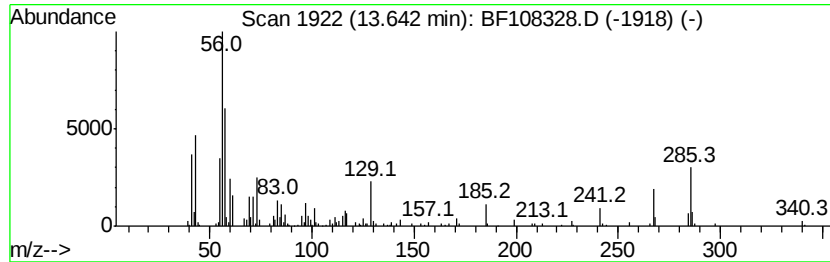
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Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	4.66 ng	364750	Chrysene-d12	14.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	90
2		Butyl myristate	284	C18H36O2	000110-36-1	72
3		Octadecanoic acid, 2-methylpropyl ester	340	C22H44O2	000646-13-9	47
4		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38



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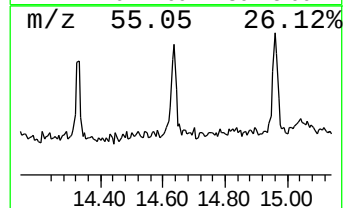
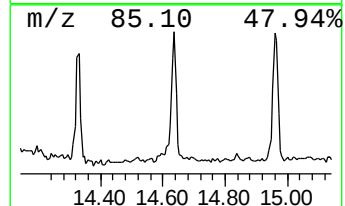
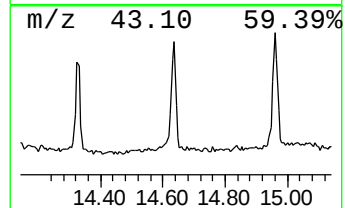
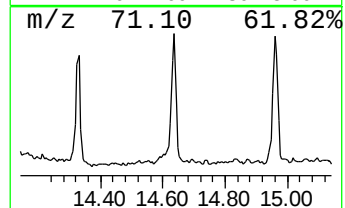
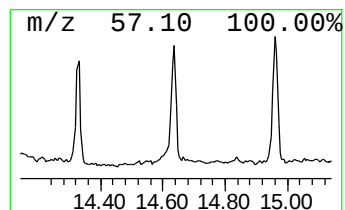
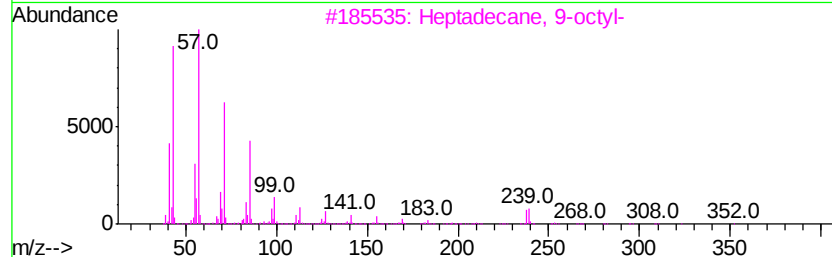
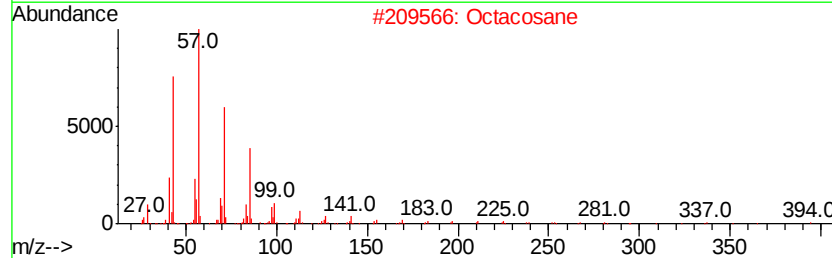
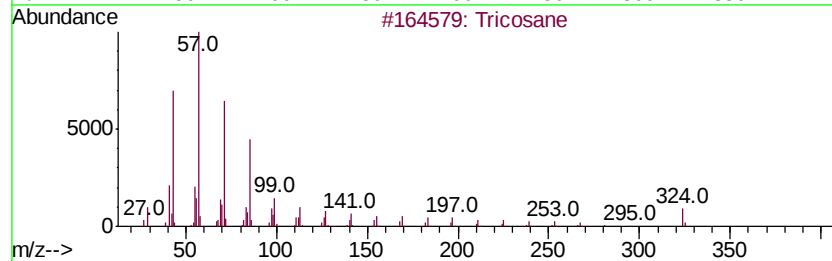
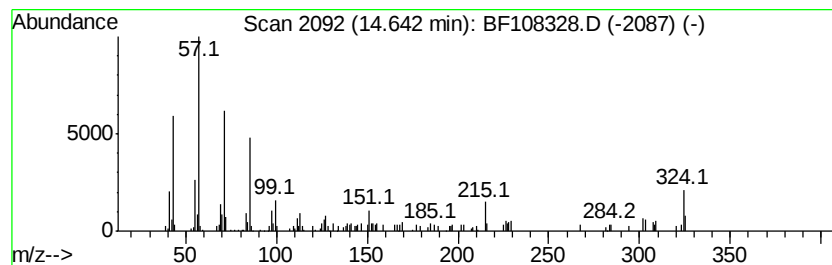
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Peak Number 6 Tricosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.32 ng	181812	Chrysene-d12	14.20
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Tricosane	324 C23H48	000638-67-5	94
2	Octacosane	394 C28H58	000630-02-4	90
3	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	87
4	Tetracosane	338 C24H50	000646-31-1	87
5	2-methyloctacosane	408 C29H60	1000376-72-8	87



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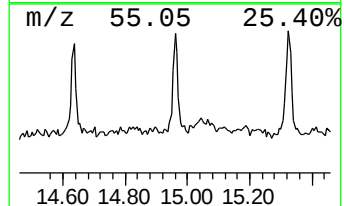
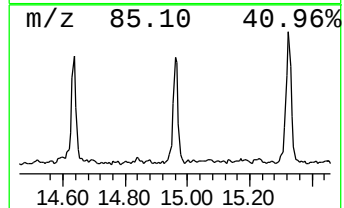
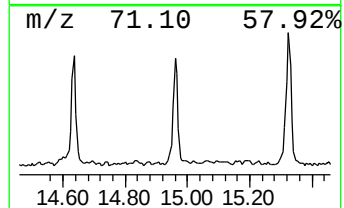
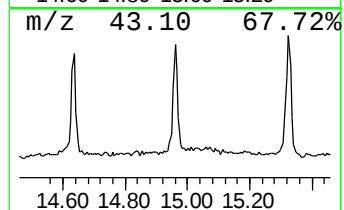
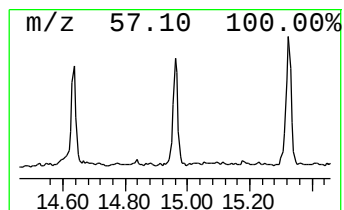
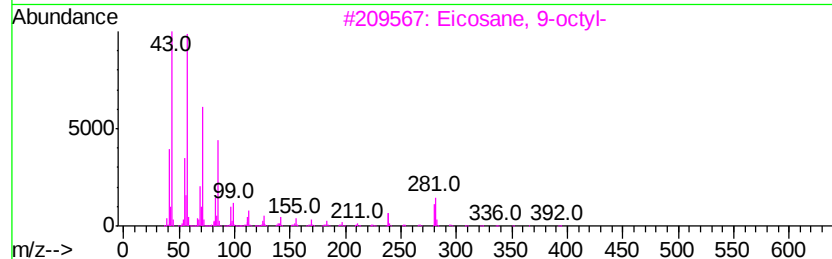
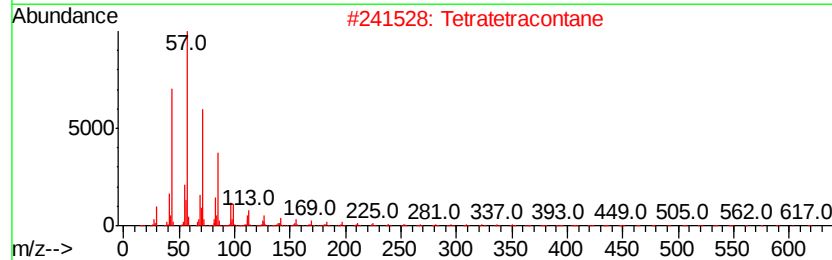
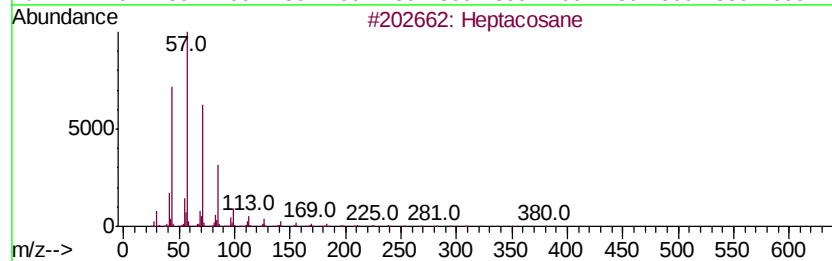
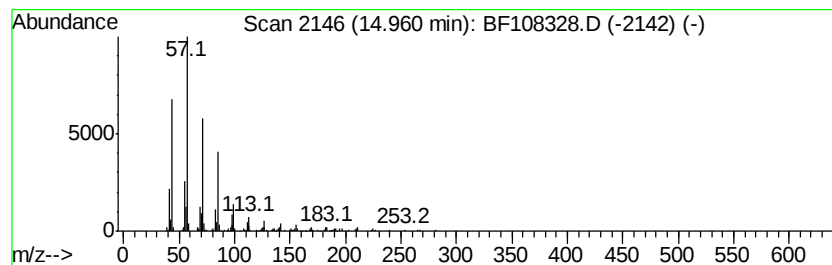
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 Heptacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	2.52 ng	197371	Chrysene-d12	14.20

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Tetratetracontane		619	C44H90	007098-22-8	91
3	Eicosane, 9-octyl-		394	C28H58	013475-77-9	91
4	Eicosane		282	C20H42	000112-95-8	90
5	Heneicosane		296	C21H44	000629-94-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082118\
Data File : BF108328.D
Acq On : 21 Aug 2018 10:23
Operator : JU/SJ
Sample : J4500-16
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7

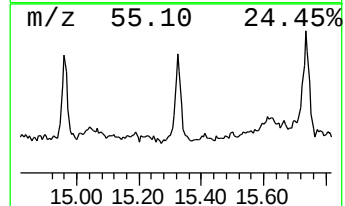
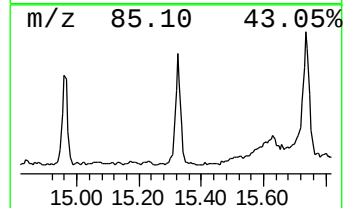
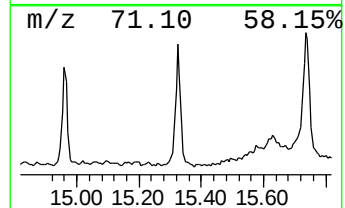
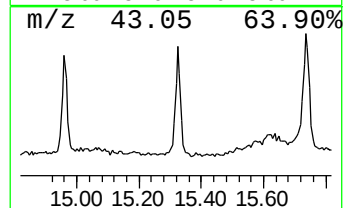
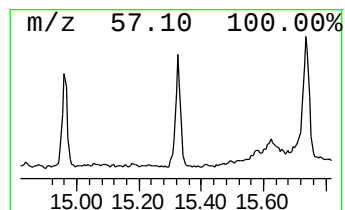
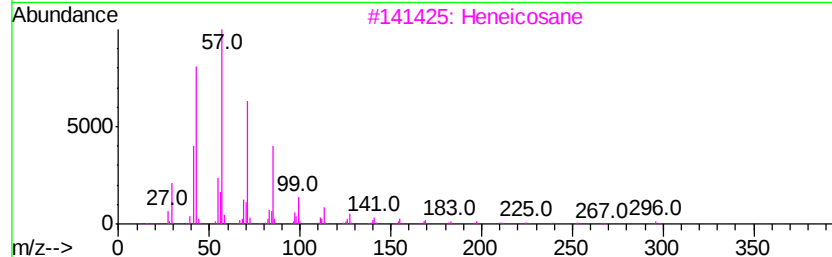
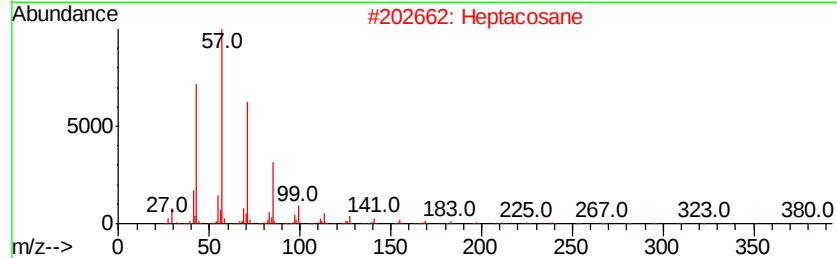
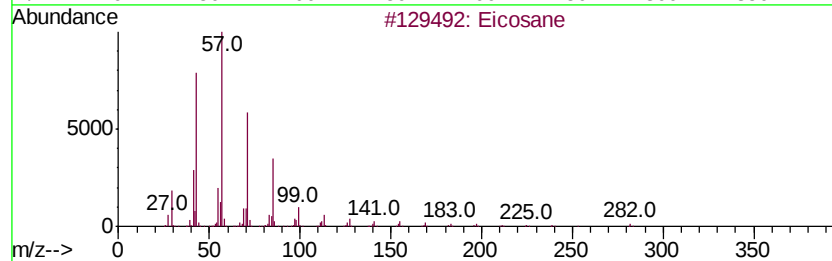
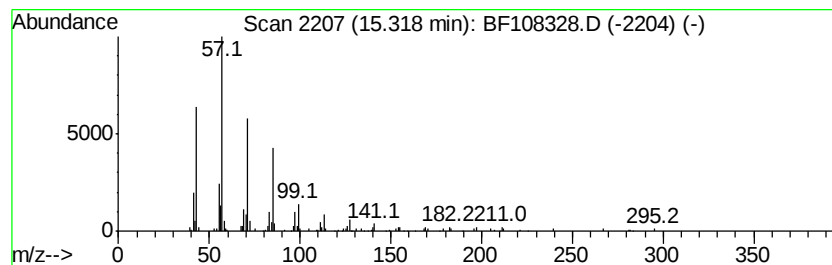
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	3.53 ng	235475	Perylene-d12	15.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	97
2		Heptacosane	380	C27H56	000593-49-7	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082118\
Data File : BF108328.D
Acq On : 21 Aug 2018 10:23
Operator : JU/SJ
Sample : J4500-16
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7

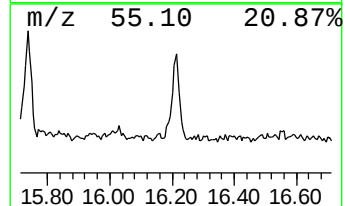
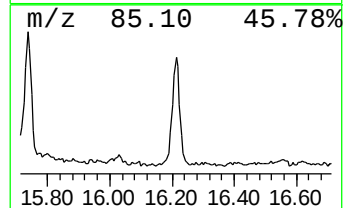
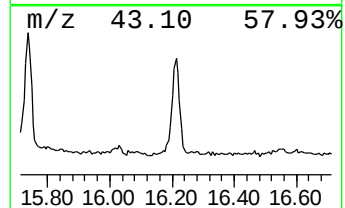
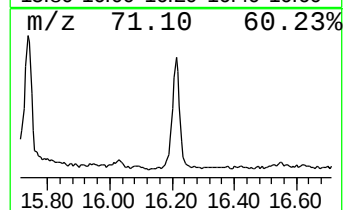
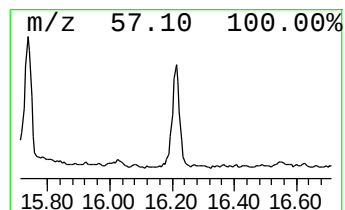
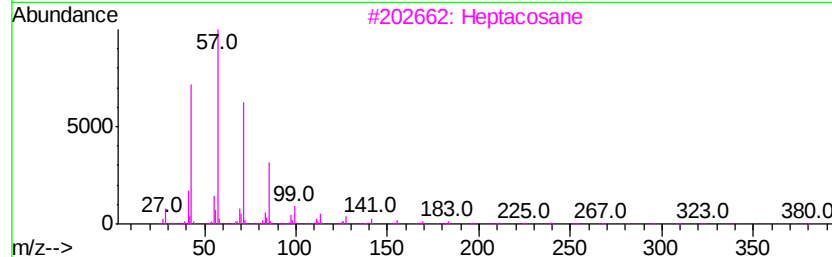
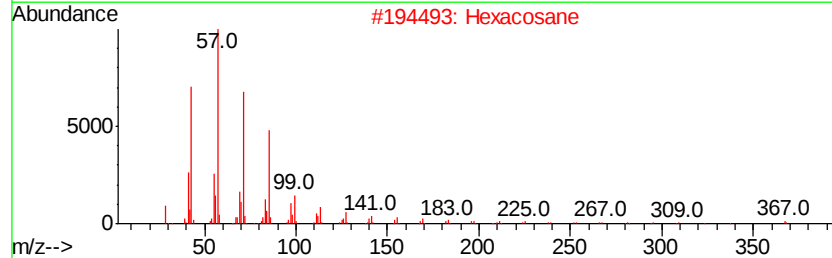
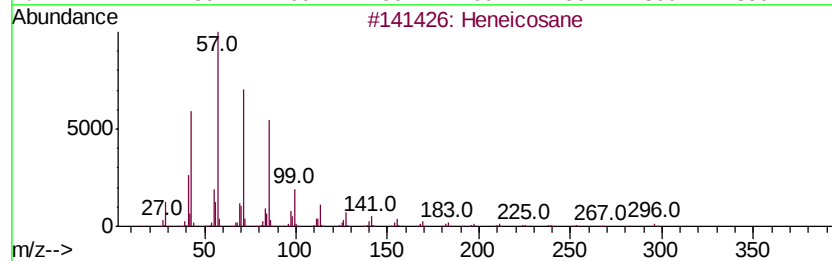
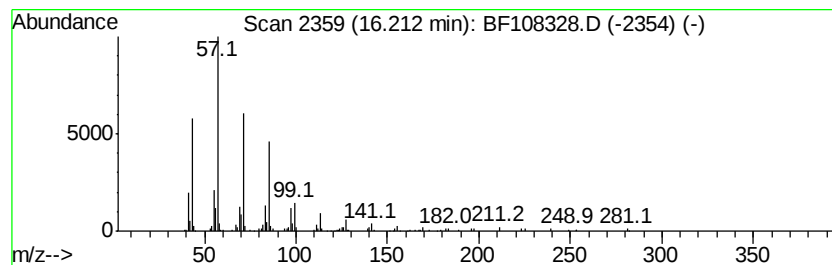
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	4.70 ng	313991	Perylene-d12	15.76

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Hexacosane		366	C26H54	000630-01-3	91
3	Heptacosane		380	C27H56	000593-49-7	90
4	Eicosane		282	C20H42	000112-95-8	87
5	Nonadecane, 2-methyl-		282	C20H42	001560-86-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082118\
Data File : BF108328.D
Acq On : 21 Aug 2018 10:23
Operator : JU/SJ
Sample : J4500-16
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7

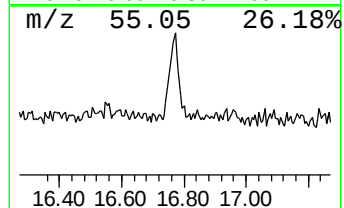
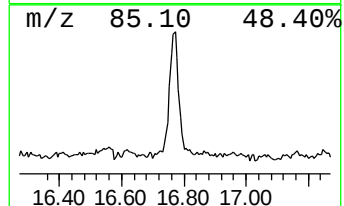
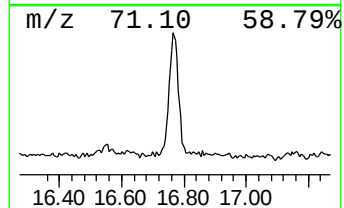
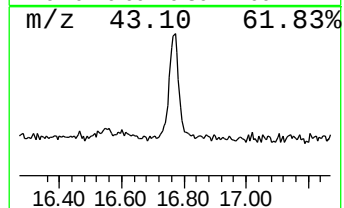
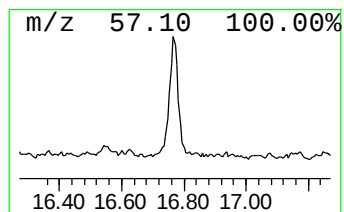
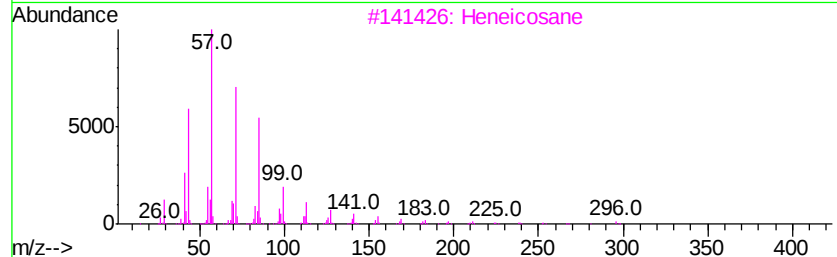
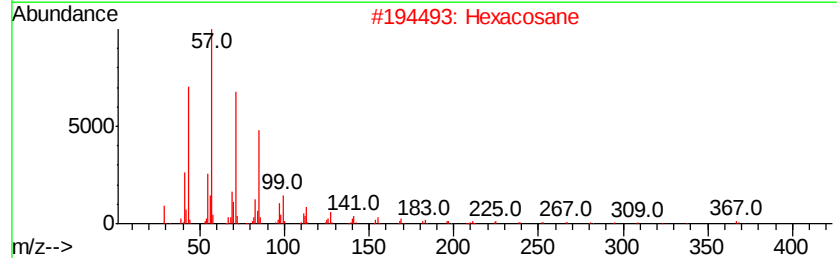
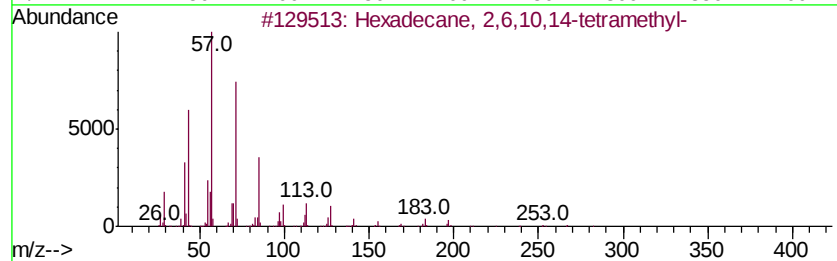
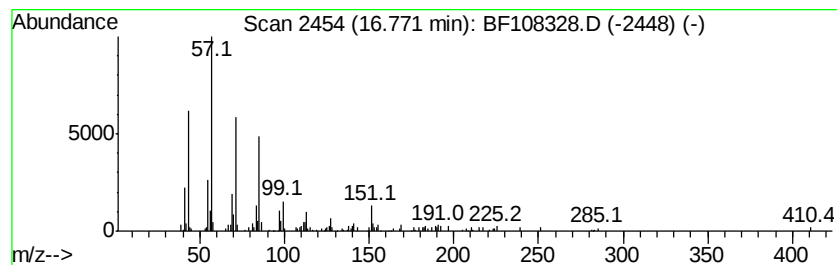
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecane, 2,6,10,14-tetra... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.77	3.47 ng	231345	Perylene-d12	15.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
2			Hexacosane	366	C26H54	000630-01-3	87
3			Heneicosane	296	C21H44	000629-94-7	87
4			Tetratetracontane	619	C44H90	007098-22-8	87
5			Hexatriacontane	507	C36H74	000630-06-8	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082118\
Data File : BF108328.D
Acq On : 21 Aug 2018 10:23
Operator : JU/SJ
Sample : J4500-16
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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...	5.28	16.9	ng	927935	1	7.01	1099280	20.0
unknown6.78	6.78	97.2	ng	5344250	1	7.01	1099280	20.0
Hexadecanoic acid...	12.93	6.0	ng	473527	5	14.20	1564970	20.0
Octadecanoic acid...	13.64	4.7	ng	364750	5	14.20	1564970	20.0
Tricosane	14.64	2.3	ng	181812	5	14.20	1564970	20.0
Heptacosane	14.96	2.5	ng	197371	5	14.20	1564970	20.0
Eicosane	15.32	3.5	ng	235475	6	15.76	1335190	20.0
Heneicosane	16.21	4.7	ng	313991	6	15.76	1335190	20.0
Hexadecane, 2,6,1...	16.77	3.5	ng	231345	6	15.76	1335190	20.0