

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
 Data File : BF102254.D
 Acq On : 20 Jan 2018 10:01
 Operator : SJ/JU
 Sample : J1114-19
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-30-2.5-3.0

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:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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	4.934	479	484	495	rVB	209109	335445	7.84%	0.873%
2	5.334	547	552	555	rBV	3542645	4225742	98.77%	10.998%
3	6.363	721	727	730	rBV	3425529	4278171	100.00%	11.135%
4	6.492	744	749	752	rBV	4108456	4227391	98.81%	11.002%
5	6.716	784	787	791	rBV	1019370	809315	18.92%	2.106%
6	6.875	809	814	817	rBV	3489556	3224325	75.37%	8.392%
7	7.287	878	884	887	rBV	2615900	2753346	64.36%	7.166%
8	7.998	1001	1005	1008	rBV	1313060	1081436	25.28%	2.815%
9	9.081	1183	1189	1192	rBV	3955991	4209047	98.38%	10.955%
10	9.469	1251	1255	1258	rBV	390098	312616	7.31%	0.814%
11	9.681	1282	1291	1296	rBV	94559	101117	2.36%	0.263%
12	9.751	1299	1303	1307	rVB2	1317165	1160529	27.13%	3.020%
13	10.180	1369	1376	1380	rBV2	137445	147093	3.44%	0.383%
14	10.545	1431	1438	1441	rBV	2538657	2669857	62.41%	6.949%
15	10.657	1453	1457	1463	rBV	105710	111556	2.61%	0.290%
16	11.233	1551	1555	1559	rBV	1319575	1148836	26.85%	2.990%
17	12.645	1791	1795	1798	rBV	189850	153872	3.60%	0.400%
18	12.722	1805	1808	1811	rVB	52461	45382	1.06%	0.118%
19	12.827	1820	1826	1829	rBV	3762212	3807542	89.00%	9.910%
20	13.304	1897	1907	1911	rBV	58049	78975	1.85%	0.206%
21	13.351	1911	1915	1917	rBV	123791	110877	2.59%	0.289%
22	13.716	1973	1977	1980	rBV	651267	683858	15.98%	1.780%
23	13.745	1980	1982	1987	rVB	96300	86772	2.03%	0.226%
24	13.868	1997	2003	2007	rBV	1202032	1109523	25.93%	2.888%
25	14.039	2029	2032	2038	rBV	61986	63106	1.48%	0.164%
26	14.345	2080	2084	2089	rBV	186789	209544	4.90%	0.545%
27	14.639	2129	2134	2141	rBV2	66586	96792	2.26%	0.252%
28	14.957	2184	2188	2191	rBV	72722	88254	2.06%	0.230%
29	15.292	2240	2245	2248	rBV	720886	840491	19.65%	2.187%
30	15.721	2314	2318	2322	rBV	51824	75784	1.77%	0.197%
31	15.774	2322	2327	2334	rVB3	60806	99530	2.33%	0.259%
32	16.198	2394	2399	2405	rBV2	42760	76401	1.79%	0.199%

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

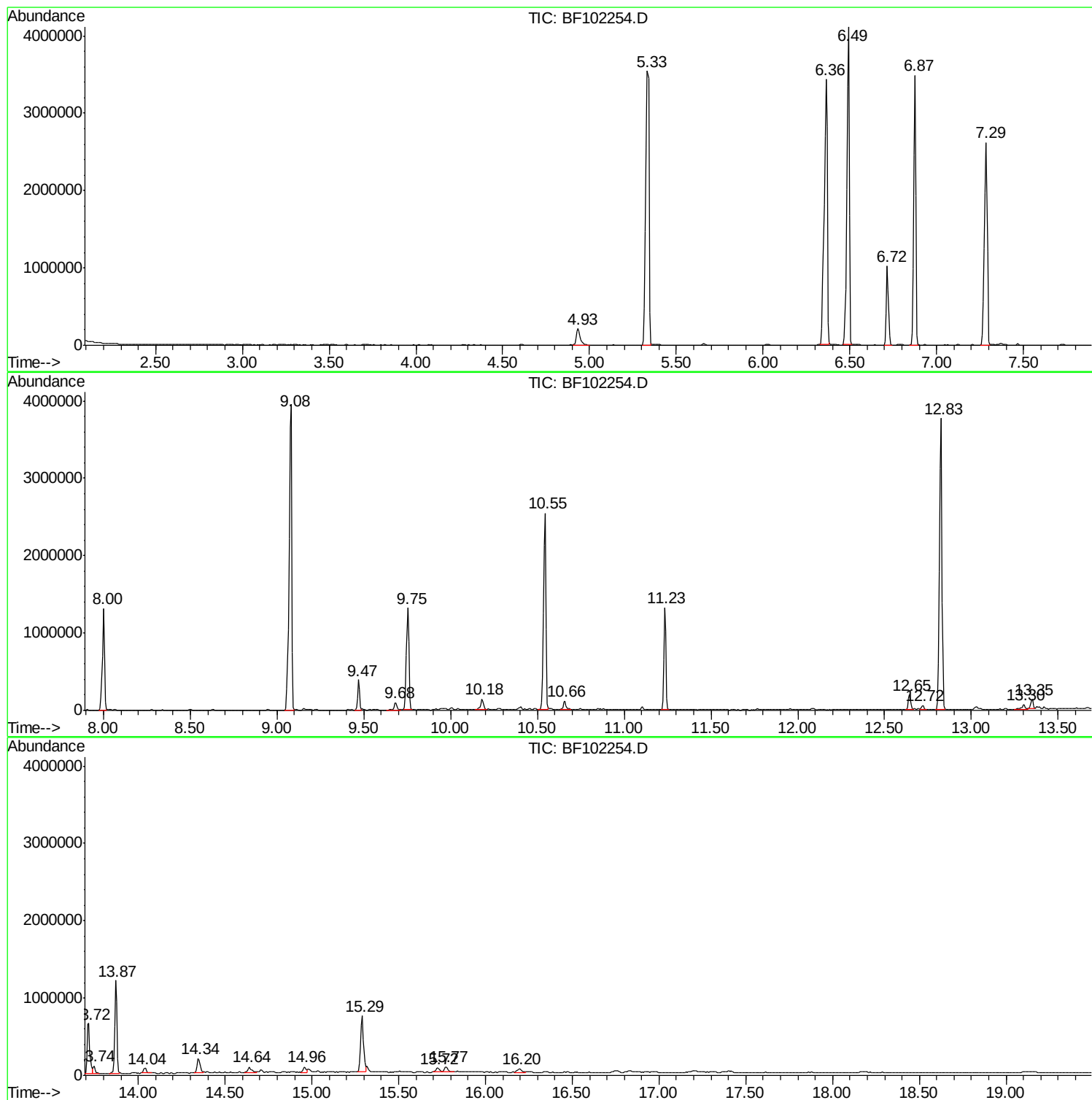
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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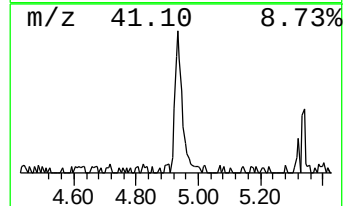
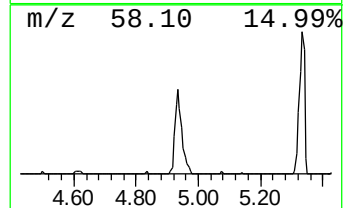
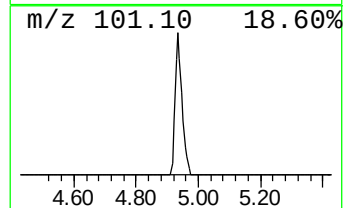
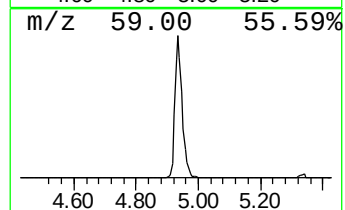
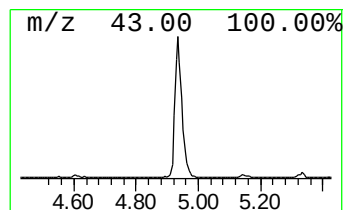
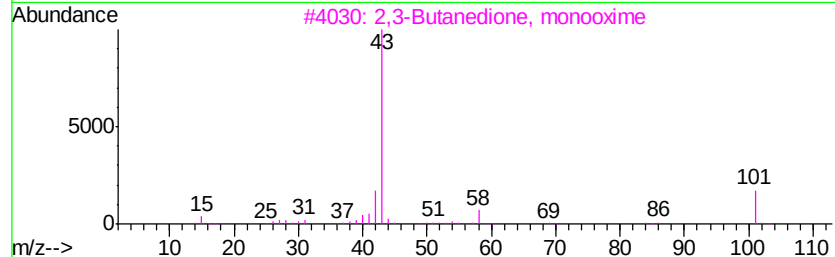
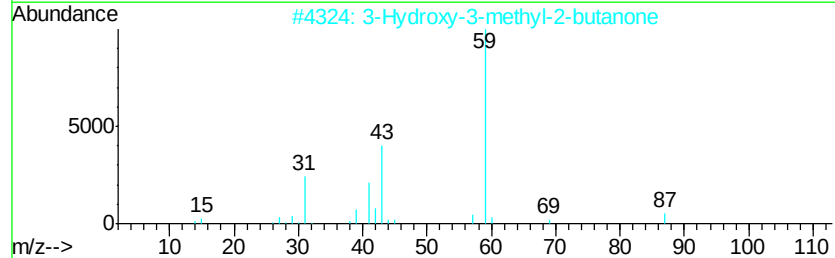
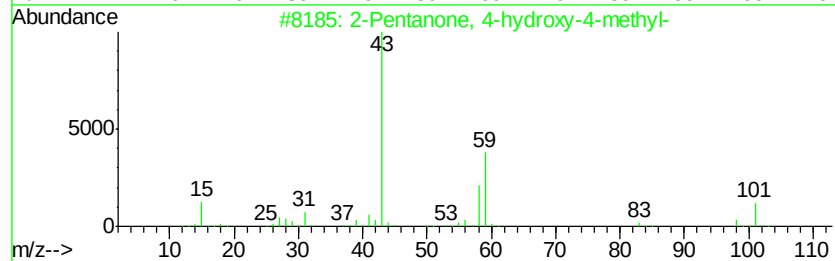
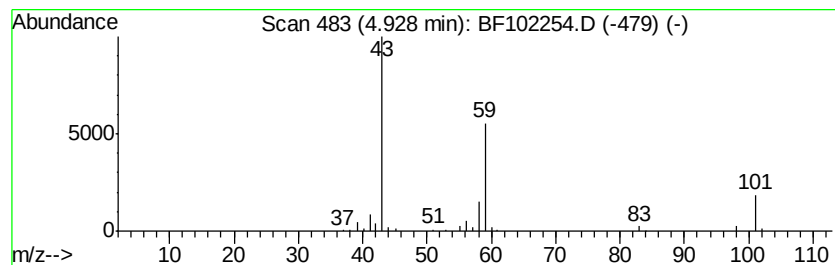
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	8.29 ng	335445	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	72		
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
4	1,2-Butanediol	90	C4H10O2	000584-03-2	9		
5	2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	9		



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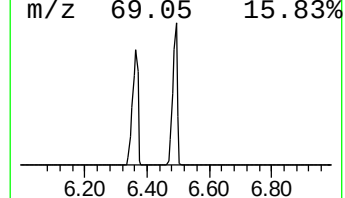
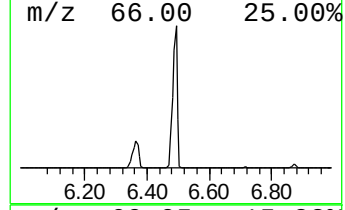
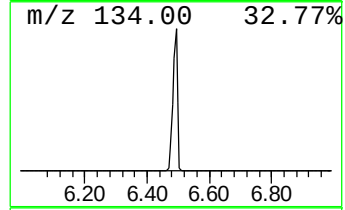
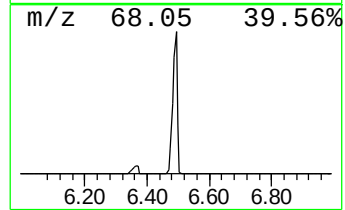
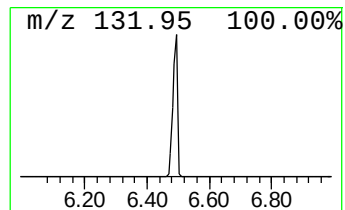
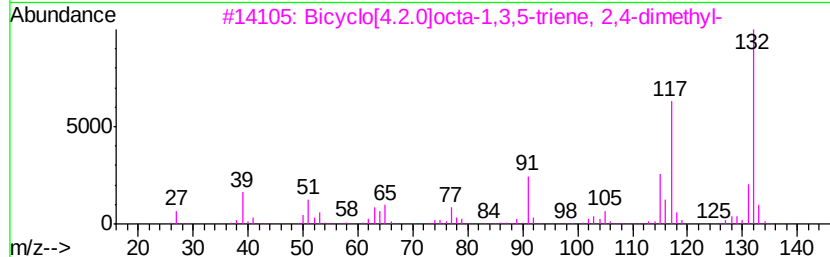
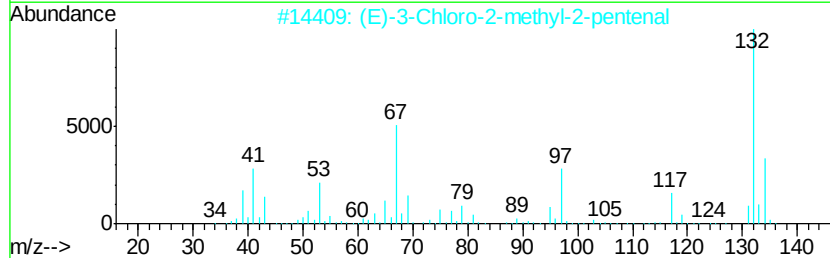
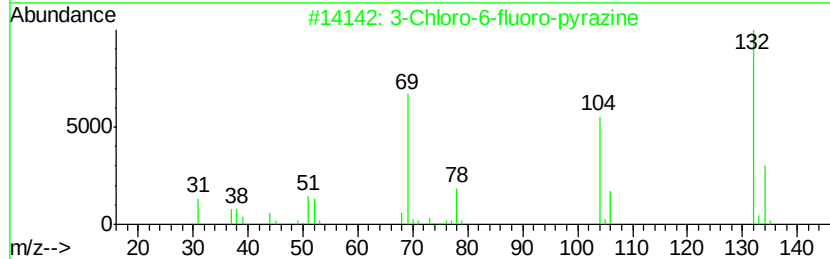
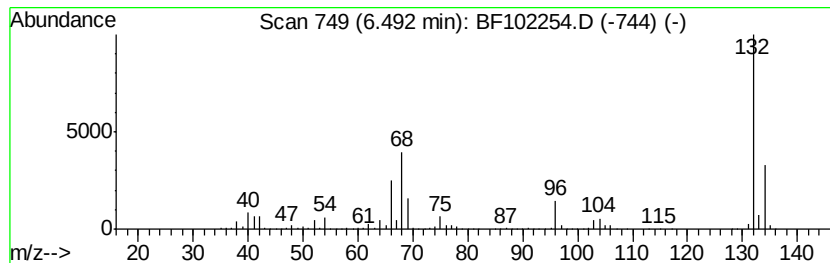
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	104.47 ng	4227390	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		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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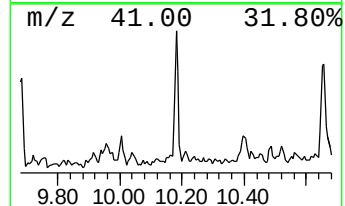
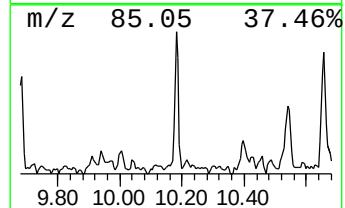
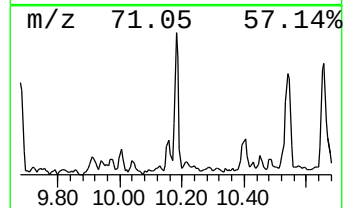
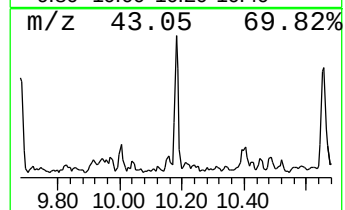
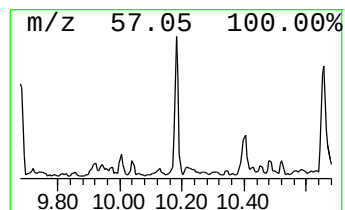
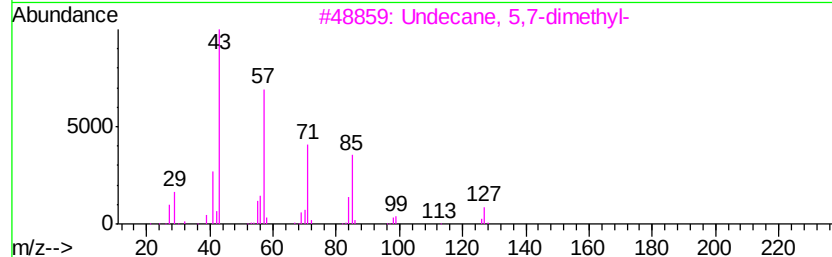
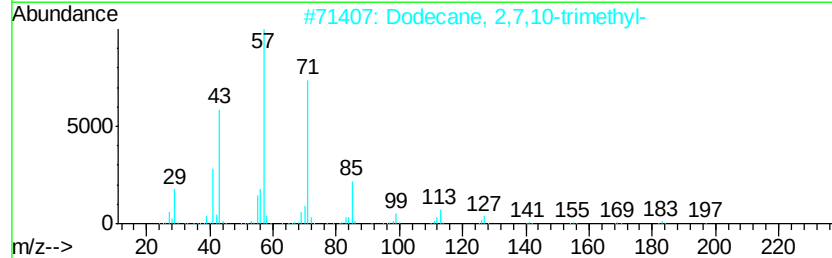
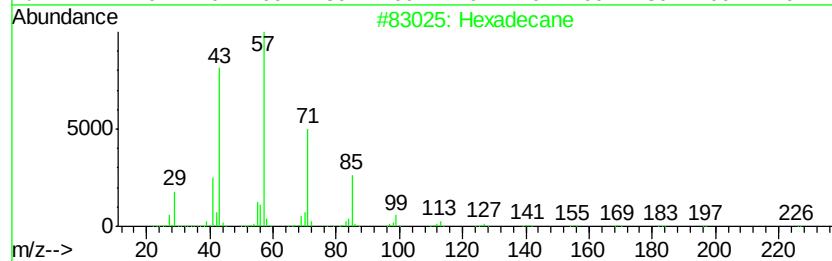
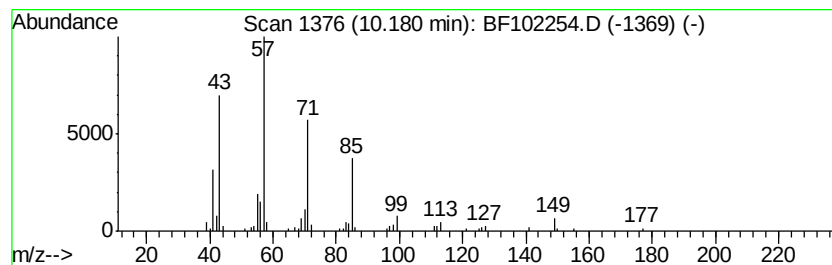
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.18	2.53 ng	147093	Acenaphthene-d10	9.75	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
3	Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3	72
4	Undecane, 6-ethyl-	184	C13H28	017312-60-6	72
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	64



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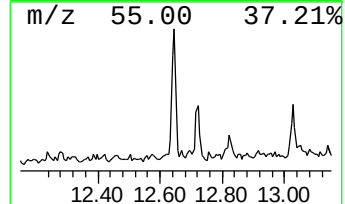
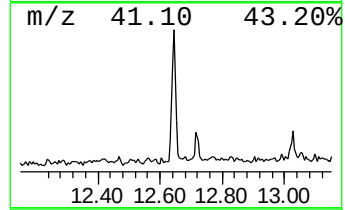
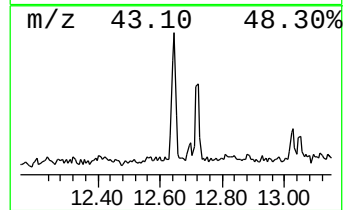
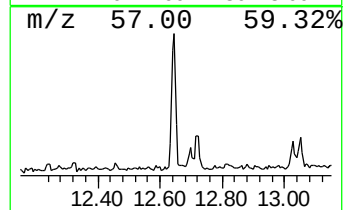
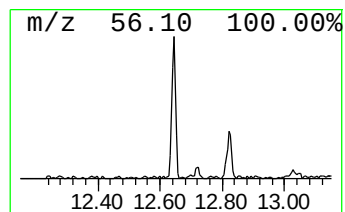
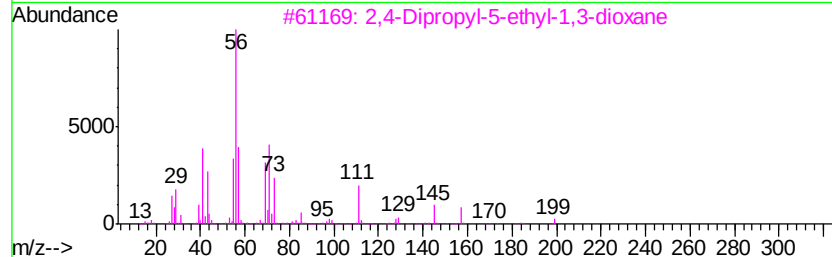
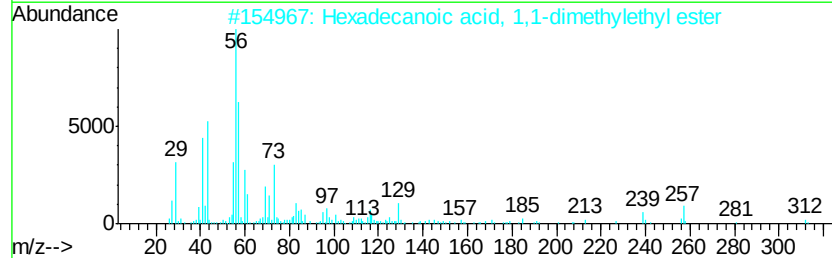
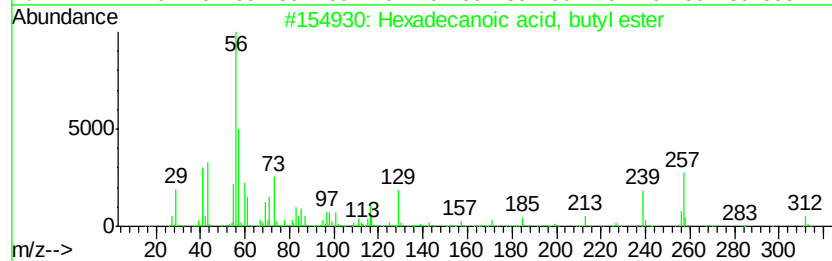
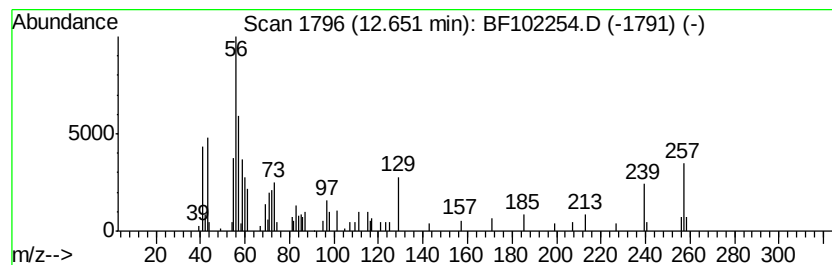
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.77 ng	153872	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	38
3		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	38
4		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	35
5		1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	32



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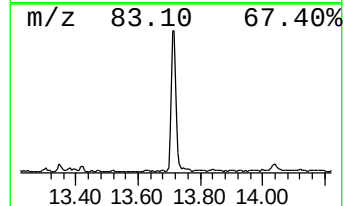
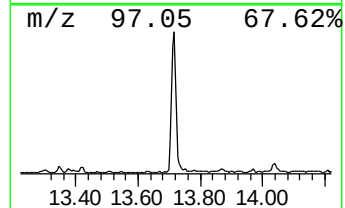
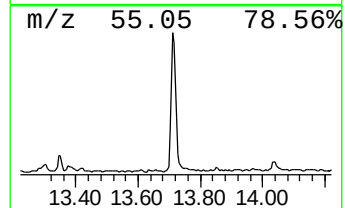
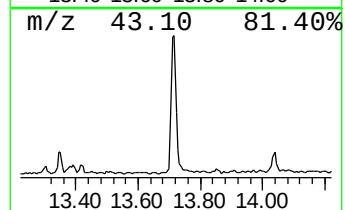
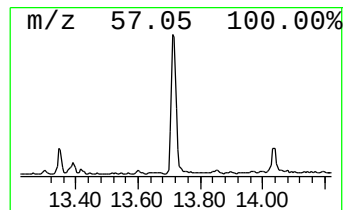
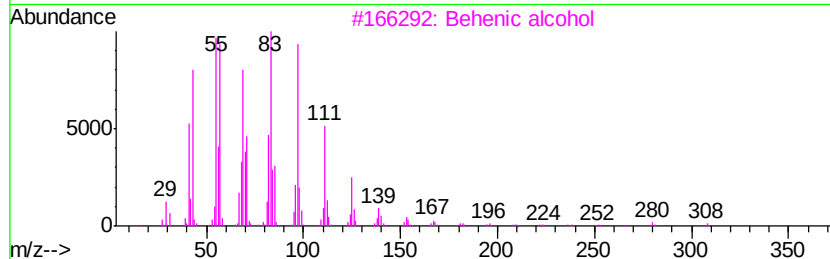
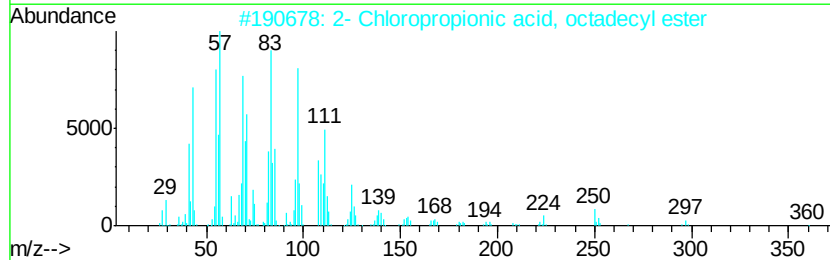
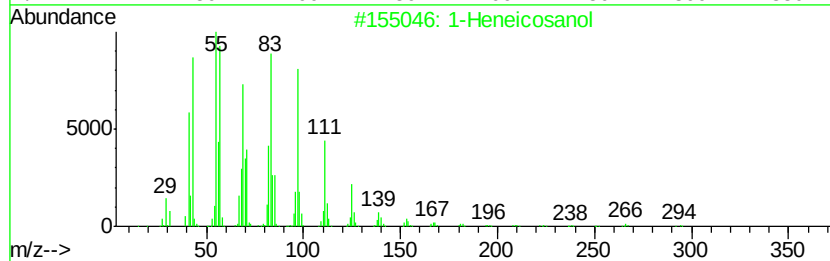
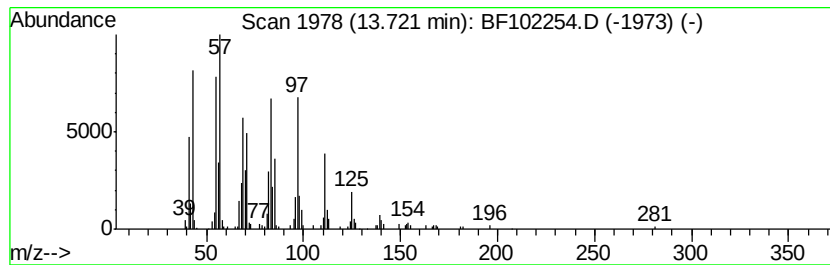
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Peak Number 6 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.72	12.33 ng	683858	Chrysene-d12	13.87		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
3		Behenic alcohol	326	C22H46O	000661-19-8	94
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



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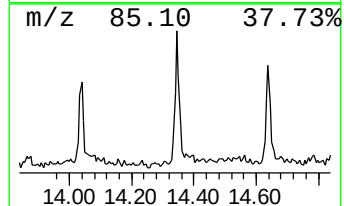
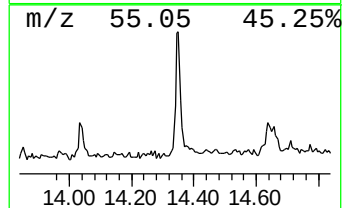
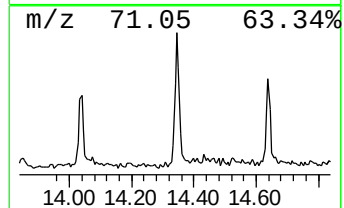
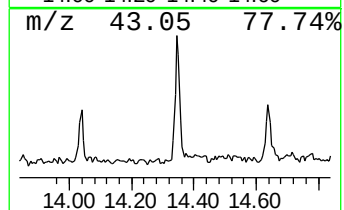
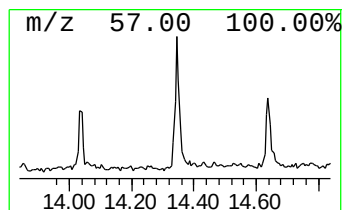
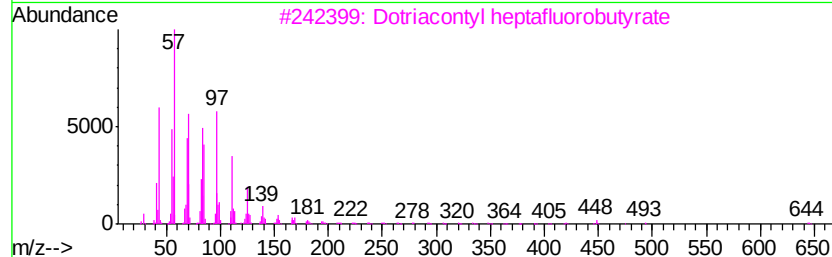
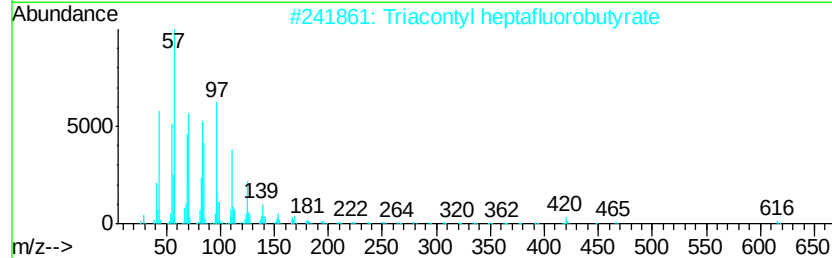
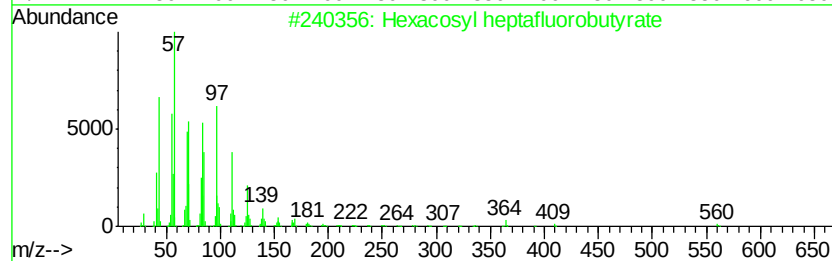
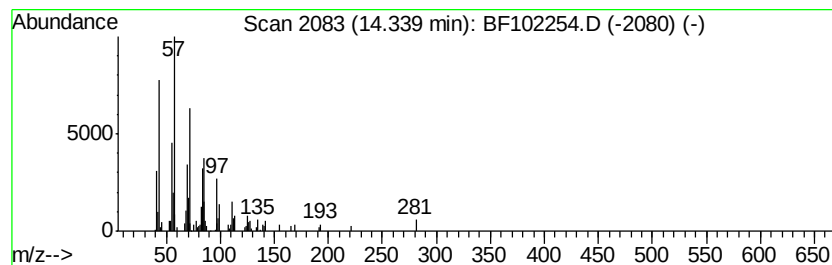
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	3.78 ng	209544	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	91
2		Triaccontyl heptafluorobutyrate	634	C34H61F7O2	1000351-83-2	91
3		Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	91
4		Triaccontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	91
5		Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
Data File : BF102254.D
Acq On : 20 Jan 2018 10:01
Operator : SJ/JU
Sample : J1114-19
Misc :
ALS Vial : 4 Sample Multiplier: 1

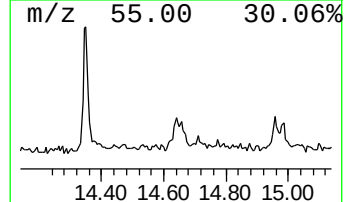
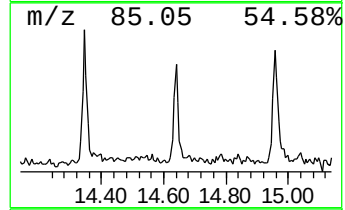
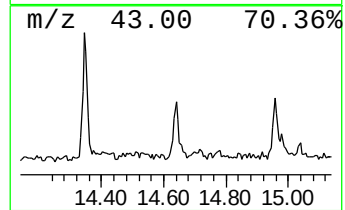
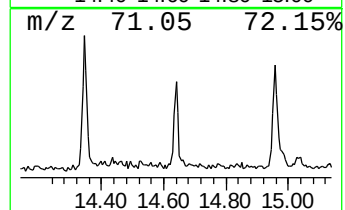
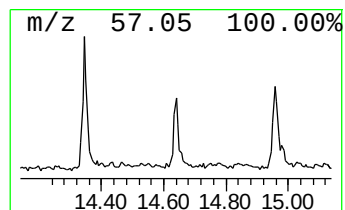
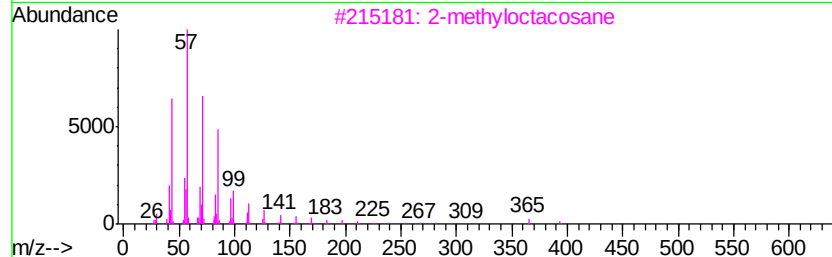
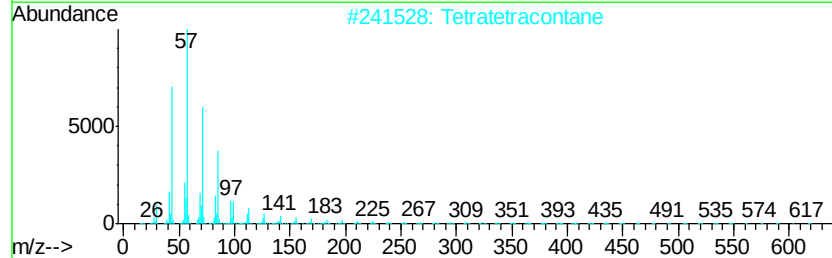
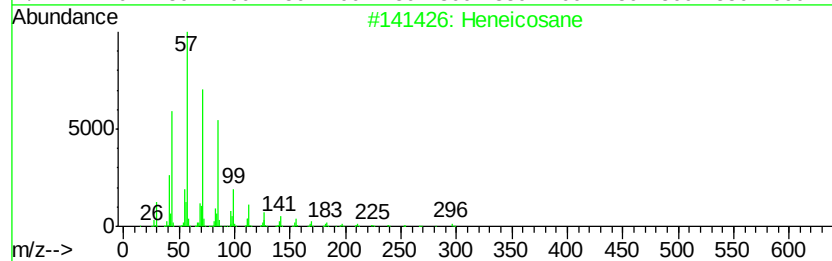
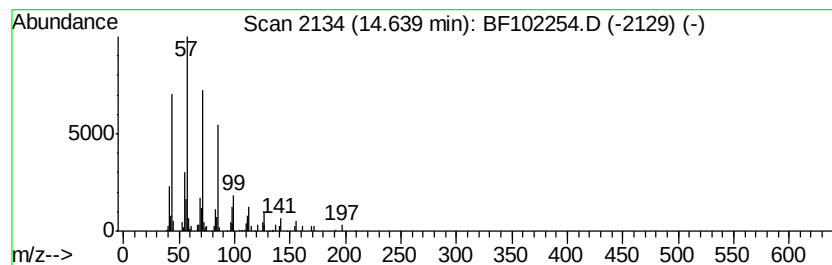
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ClientSampleId :
SB-30-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.64	2.30 ng	96792	Perylene-d12		15.29
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Octacosane	394	C28H58	000630-02-4	91
5	triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102254.D
Acq On : 20 Jan 2018 10:01
Operator : SJ/JU
Sample : J1114-19
Misc :
ALS Vial : 4 Sample Multiplier: 1

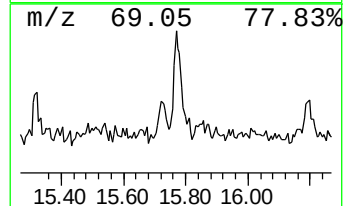
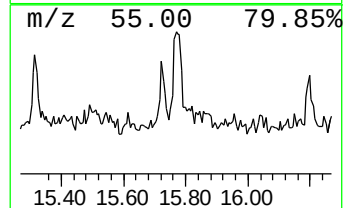
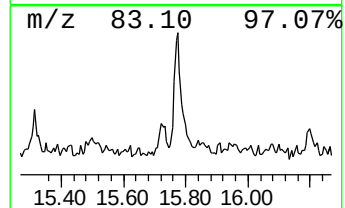
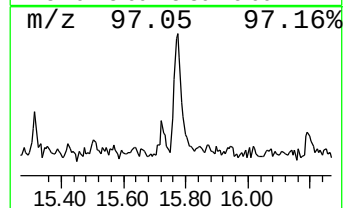
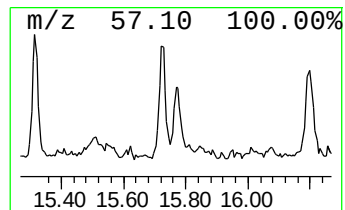
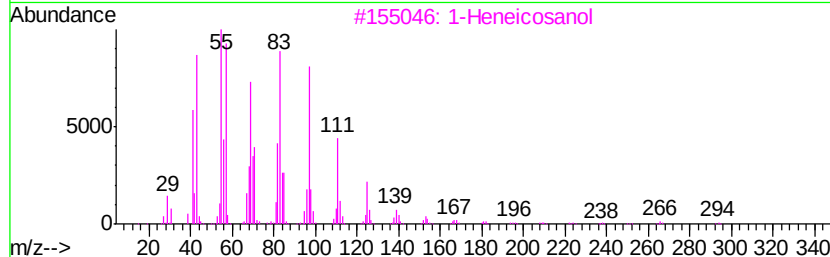
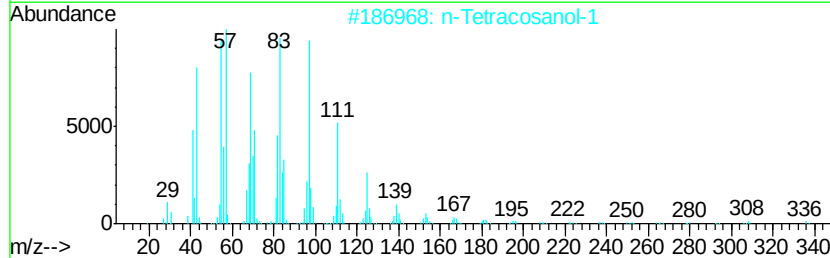
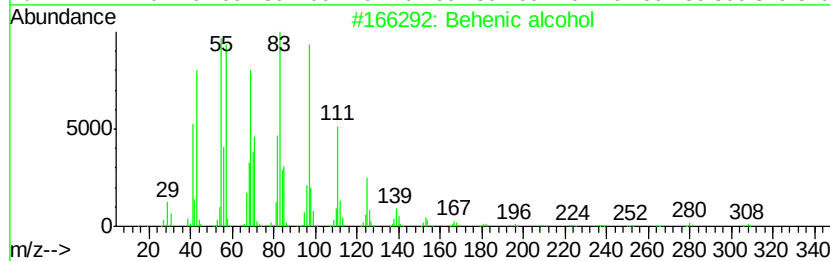
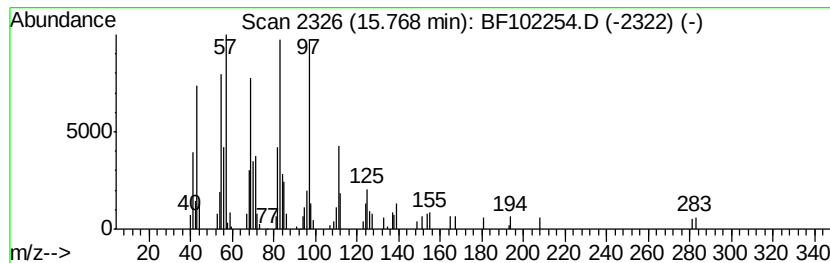
Instrument :
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ClientSampleId :
SB-30-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Behenic alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	2.37 ng	99530	Perylene-d12	15.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Behenic alcohol	326 C22H46O	000661-19-8 94
2		n-Tetracosanol-1	354 C24H50O	000506-51-4 91
3		1-Heneicosanol	312 C21H44O	015594-90-8 91
4		1-Octadecanol	270 C18H38O	000112-92-5 90
5		Octacosanol	410 C28H58O	000557-61-9 90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
Data File : BF102254.D
Acq On : 20 Jan 2018 10:01
Operator : SJ/JU
Sample : J1114-19
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-30-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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...	4.93	8.3	ng	335445	1	6.72	809315	20.0
unknown6.49	6.49	104.5	ng	4227390	1	6.72	809315	20.0
Hexadecane	10.18	2.5	ng	147093	3	9.75	1160530	20.0
Hexadecanoic acid...	12.65	2.8	ng	153872	5	13.87	1109520	20.0
1-Heneicosanol	13.72	12.3	ng	683858	5	13.87	1109520	20.0
Hexacosyl heptafl...	14.34	3.8	ng	209544	5	13.87	1109520	20.0
Heneicosane	14.64	2.3	ng	96792	6	15.29	840491	20.0
Behenic alcohol	15.77	2.4	ng	99530	6	15.29	840491	20.0