

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
 Data File : BF102887.D
 Acq On : 9 Feb 2018 14:33
 Operator : SJ/JU
 Sample : J1476-05
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GL-WC-03

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:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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	2.163	7	13	27	rVB	440570	614553	15.17%	1.793%
2	4.787	457	459	467	rVB	52340	63246	1.56%	0.184%
3	5.116	509	515	518	rVB	2905524	4050793	100.00%	11.816%
4	5.504	577	581	585	rVB	2365420	2130822	52.60%	6.216%
5	6.434	736	739	743	rBV	53599	50754	1.25%	0.148%
6	6.510	748	752	755	rBV	3100079	2982616	73.63%	8.701%
7	6.651	772	776	780	rBV	2786422	2615029	64.56%	7.628%
8	6.887	812	816	819	rBV	1254476	1019779	25.17%	2.975%
9	7.040	835	842	846	rBV	3019621	2910959	71.86%	8.492%
10	7.445	906	911	914	rBV	2456972	2400854	59.27%	7.003%
11	8.169	1030	1034	1037	rBV	1534516	1253911	30.95%	3.658%
12	9.239	1212	1216	1220	rBV	3352498	3241464	80.02%	9.456%
13	9.316	1226	1229	1231	rBV	59098	40930	1.01%	0.119%
14	9.381	1237	1240	1252	rVB9	22961	48297	1.19%	0.141%
15	9.498	1255	1260	1265	rBV2	41362	60510	1.49%	0.177%
16	9.633	1279	1283	1286	rBV	197150	178302	4.40%	0.520%
17	9.845	1315	1319	1323	rVB	151259	123548	3.05%	0.360%
18	9.922	1328	1332	1340	rVV	1249725	1183611	29.22%	3.453%
19	10.345	1397	1404	1407	rBV	167109	147820	3.65%	0.431%
20	10.569	1436	1442	1444	rBV	46547	62044	1.53%	0.181%
21	10.710	1463	1466	1477	rBV	985791	955375	23.58%	2.787%
22	10.822	1481	1485	1495	rVB	138948	173656	4.29%	0.507%
23	11.269	1558	1561	1563	rBV	84972	69809	1.72%	0.204%
24	11.410	1582	1585	1589	rBV	1072891	1035324	25.56%	3.020%
25	11.927	1669	1673	1681	rBV7	27180	43133	1.06%	0.126%
26	12.627	1789	1792	1796	rVB	59810	52973	1.31%	0.155%
27	12.857	1825	1831	1834	rBV	53975	54142	1.34%	0.158%
28	12.998	1850	1855	1858	rBV	2613693	2362939	58.33%	6.893%
29	13.880	2001	2005	2013	rBV	626391	631683	15.59%	1.843%
30	14.051	2030	2034	2038	rBV	1044574	991438	24.48%	2.892%
31	14.204	2056	2060	2065	rBV	42921	63479	1.57%	0.185%
32	14.327	2078	2081	2086	rBV	53481	41703	1.03%	0.122%
33	14.510	2108	2112	2119	rBV	247172	288517	7.12%	0.842%
34	14.892	2174	2177	2180	rBV	58854	65741	1.62%	0.192%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.968	2186	2190	2196	rBV	193685	208596	5.15%	0.608%
36	15.163	2219	2223	2226	rBV	280012	319232	7.88%	0.931%
37	15.539	2282	2287	2299	rBV2	681762	978056	24.14%	2.853%
38	15.757	2320	2324	2332	rVB	148406	211162	5.21%	0.616%
39	15.998	2360	2365	2369	rBV	162062	243559	6.01%	0.710%
40	16.045	2370	2373	2381	rVB2	56827	102215	2.52%	0.298%
41	16.815	2499	2504	2511	rVB2	109805	208263	5.14%	0.608%

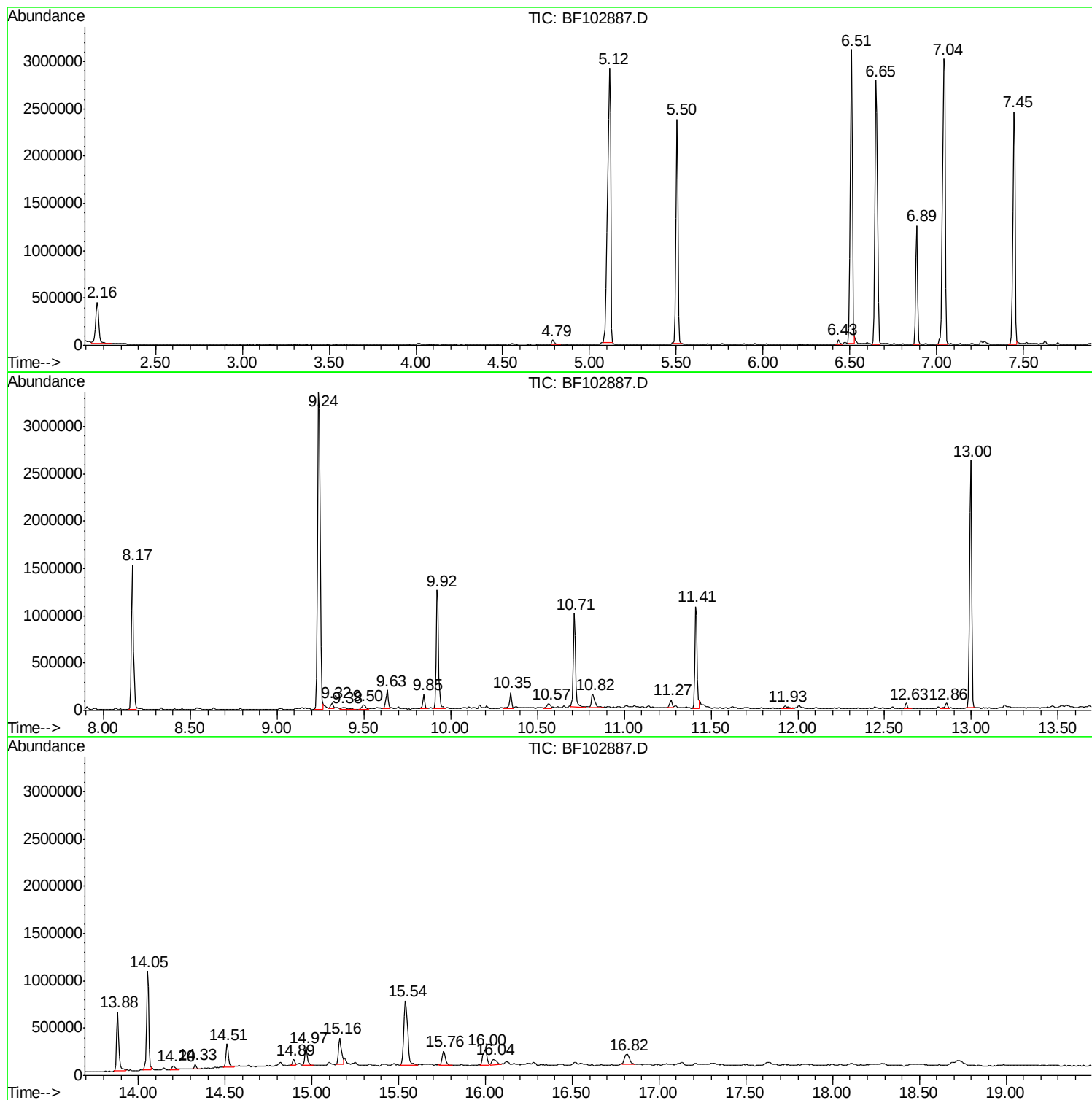
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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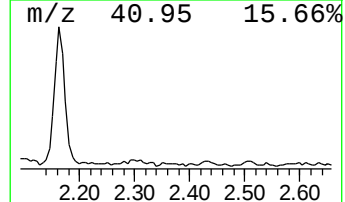
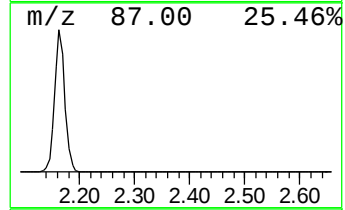
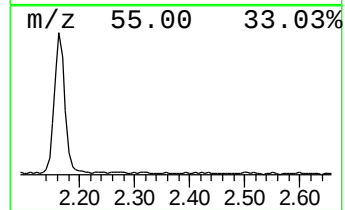
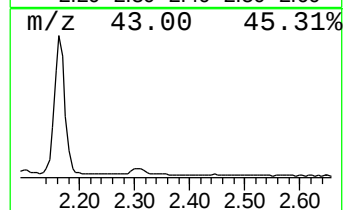
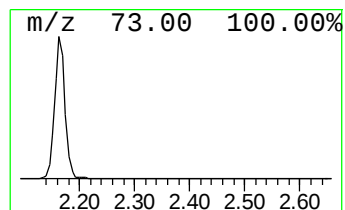
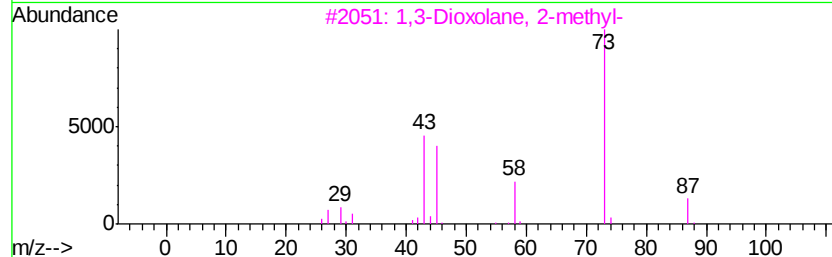
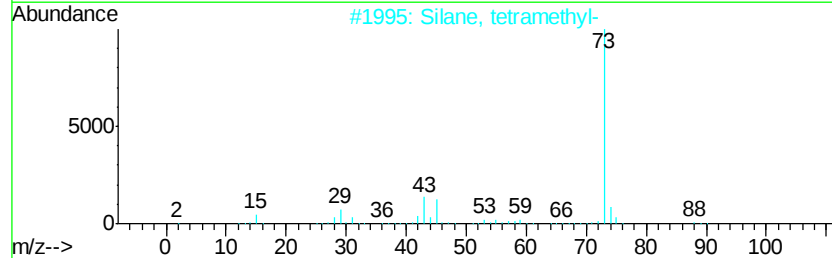
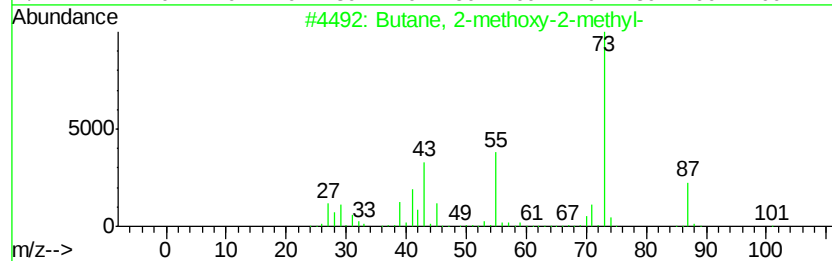
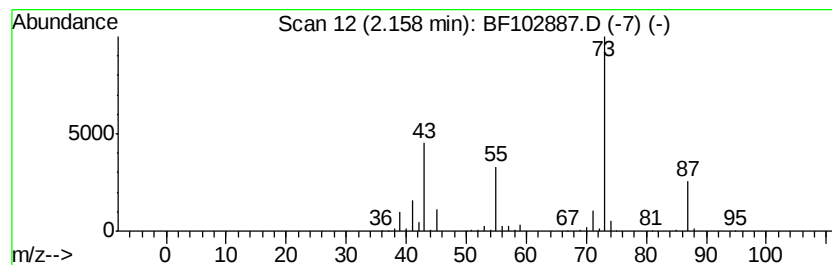
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	12.05 ng	614553	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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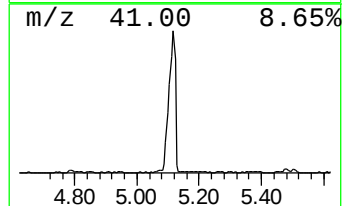
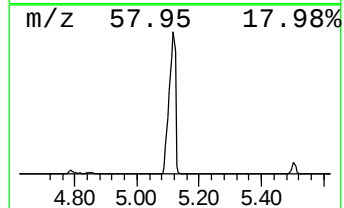
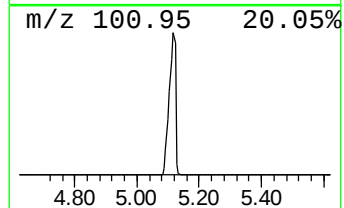
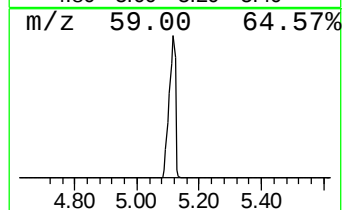
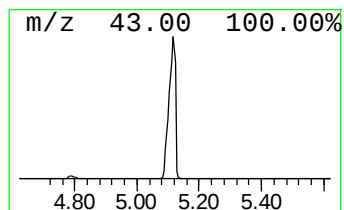
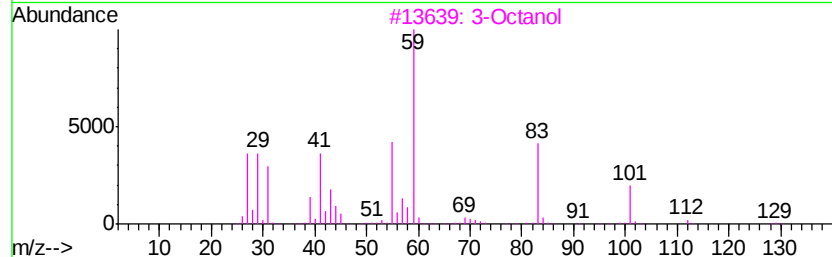
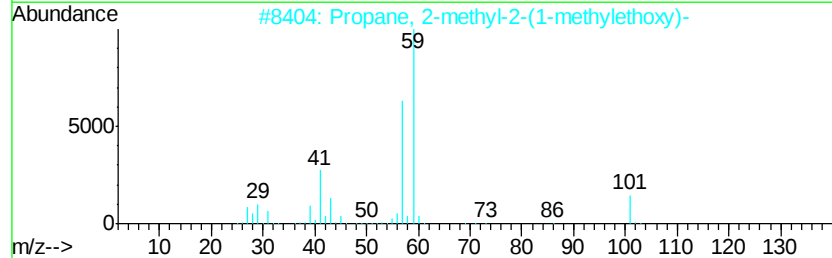
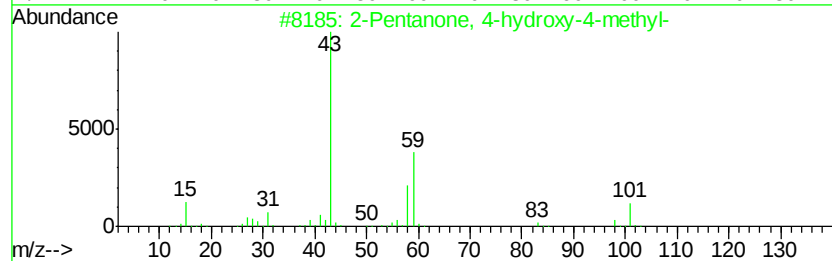
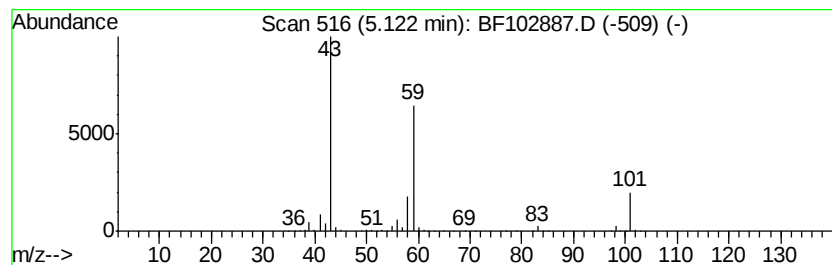
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	79.44 ng	4050790	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3			3-Octanol	130	C8H18O	000589-98-0	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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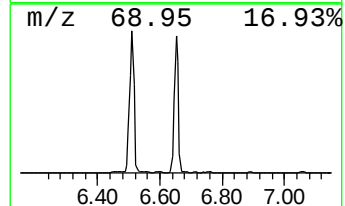
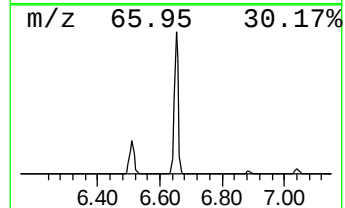
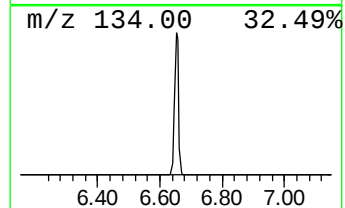
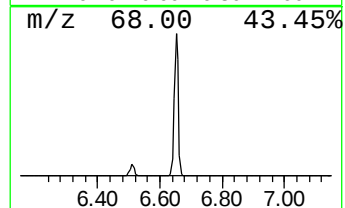
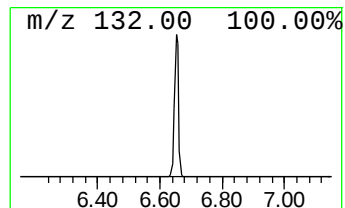
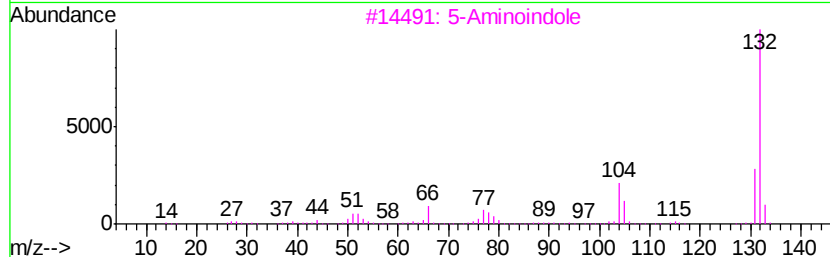
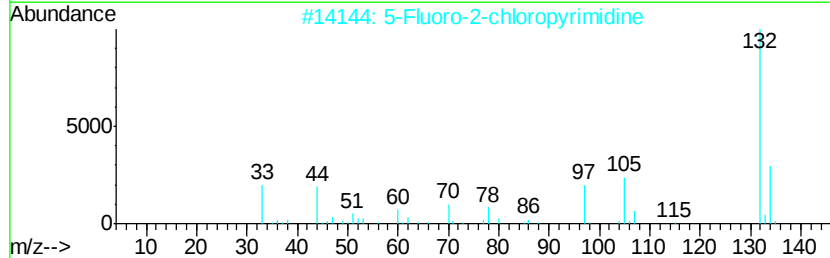
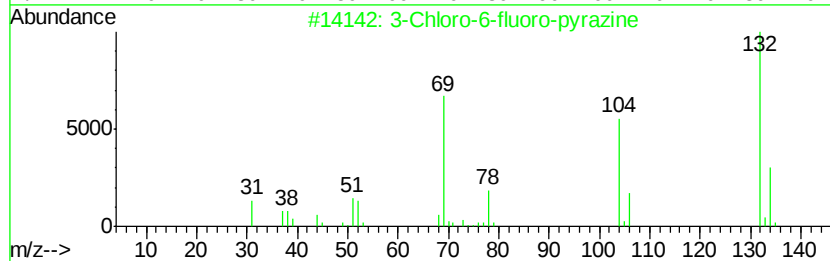
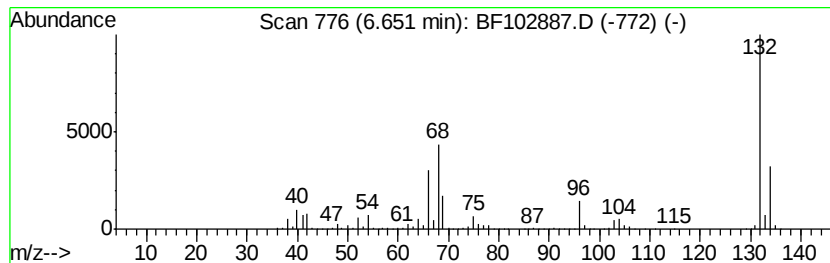
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.65 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	51.29 ng	2615030	1,4-Dichlorobenzene-d4	6.89

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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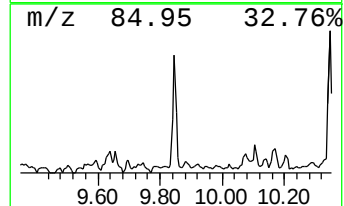
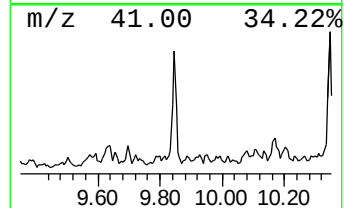
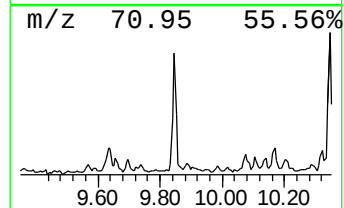
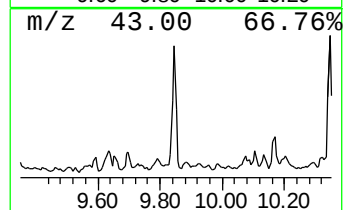
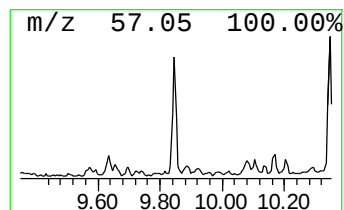
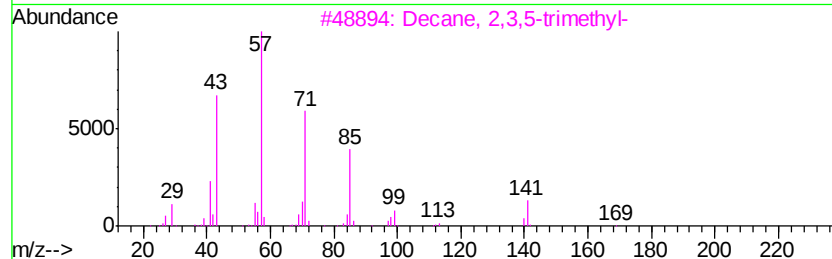
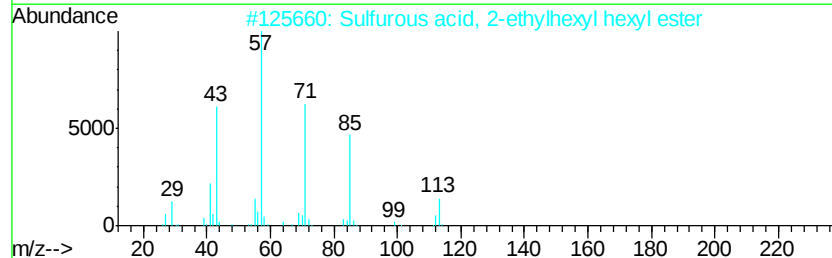
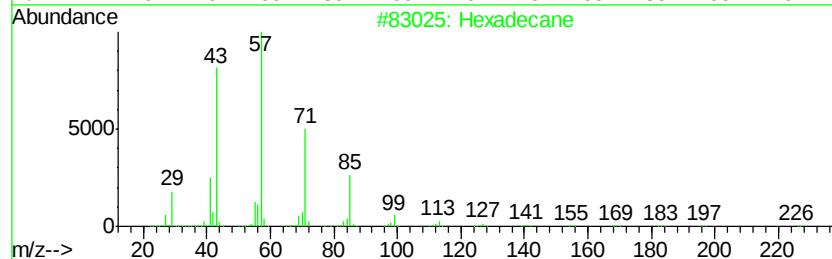
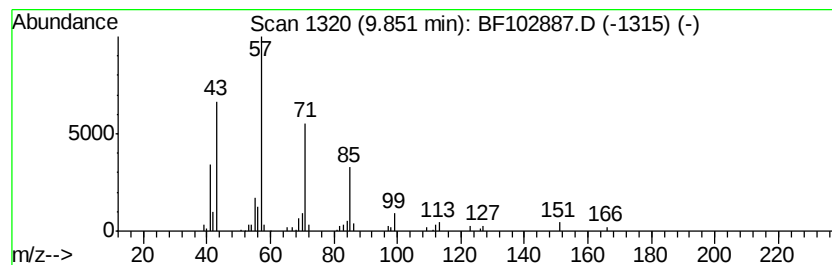
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	2.09 ng	123548	Acenaphthene-d10	9.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	91
2	Sulfurous acid, 2-ethylhexyl hex...		278	C14H30O3S	1000309-20-2	80
3	Decane, 2,3,5-trimethyl-		184	C13H28	062238-11-3	64
4	Nonadecane		268	C19H40	000629-92-5	58
5	Tetradecane		198	C14H30	000629-59-4	53



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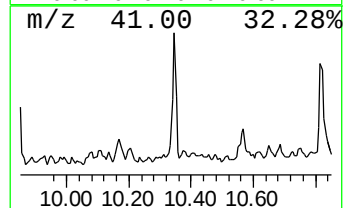
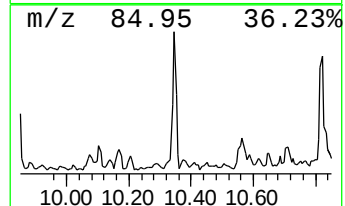
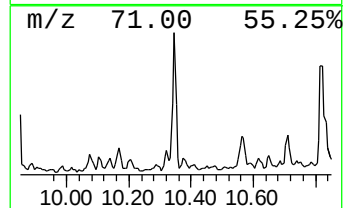
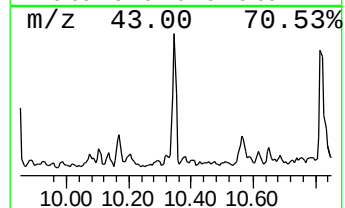
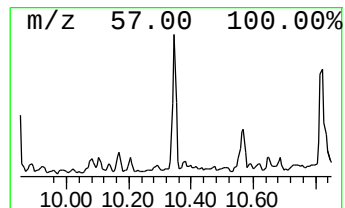
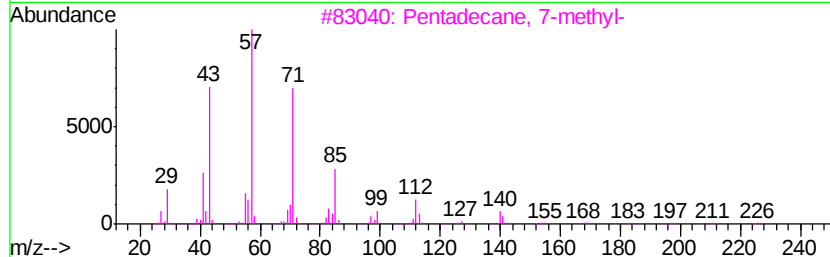
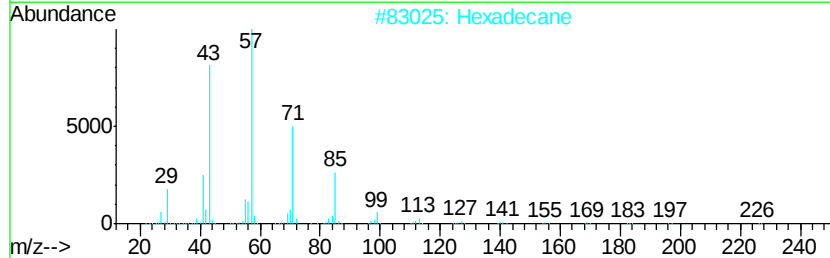
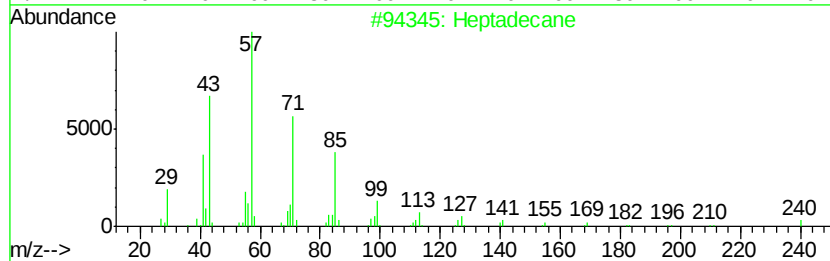
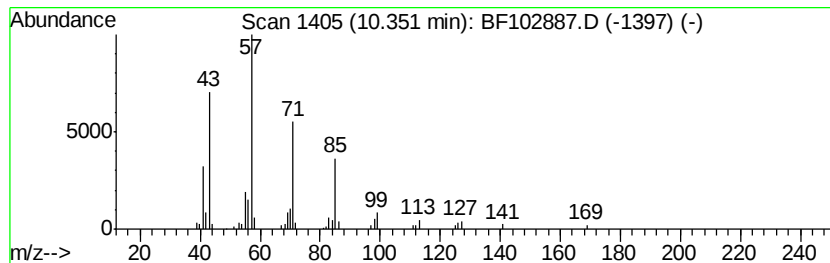
Instrument :
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.35	2.50 ng	147820	Acenaphthene-d10	9.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	83
4	Pentadecane	212	C15H32	000629-62-9	78
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102887.D
Acq On : 9 Feb 2018 14:33
Operator : SJ/JU
Sample : J1476-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

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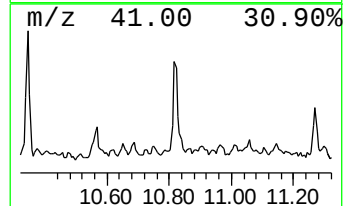
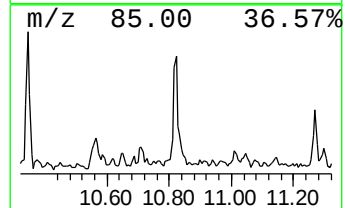
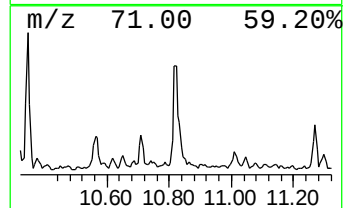
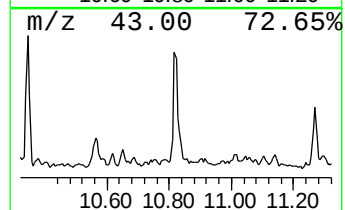
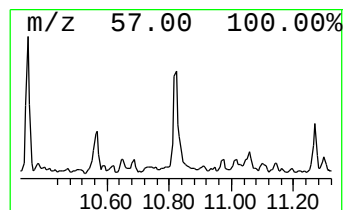
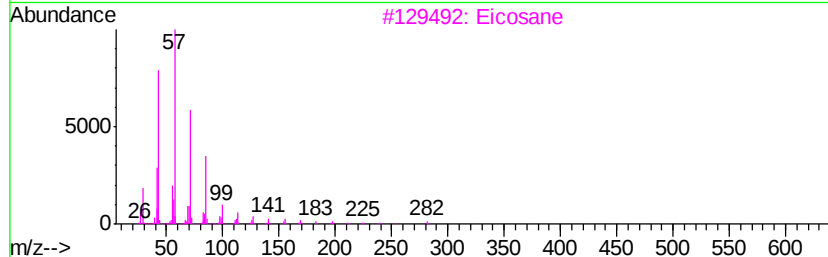
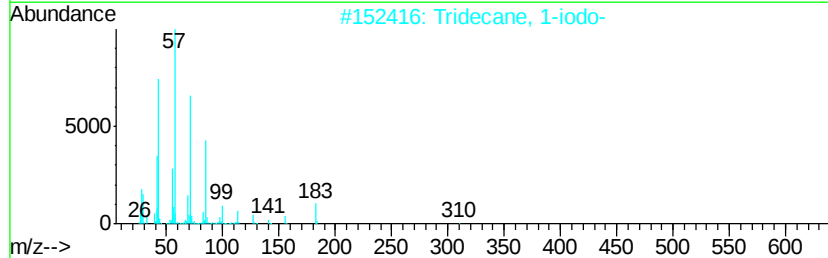
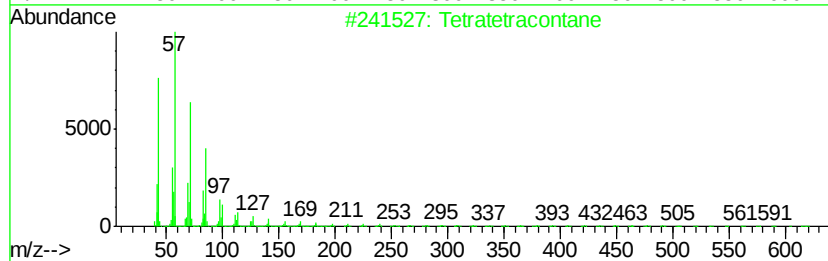
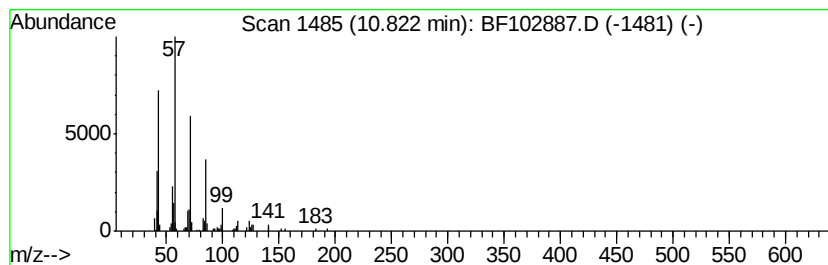
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetratetracontane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	3.35 ng	173656	Phenanthrene-d10	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	86
2		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
3		Eicosane	282	C20H42	000112-95-8	86
4		Hexadecane	226	C16H34	000544-76-3	86
5		Heptacosane	380	C27H56	000593-49-7	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102887.D
Acq On : 9 Feb 2018 14:33
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ClientSampleId :
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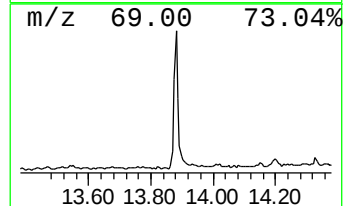
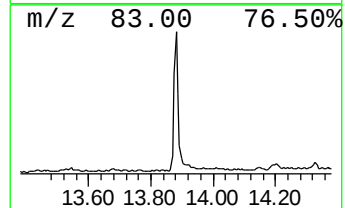
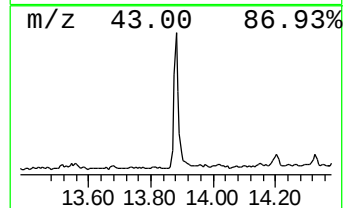
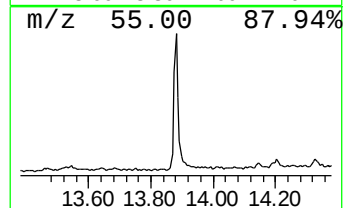
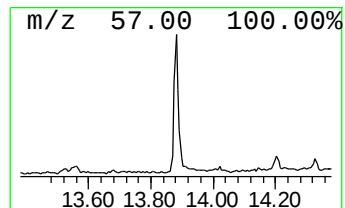
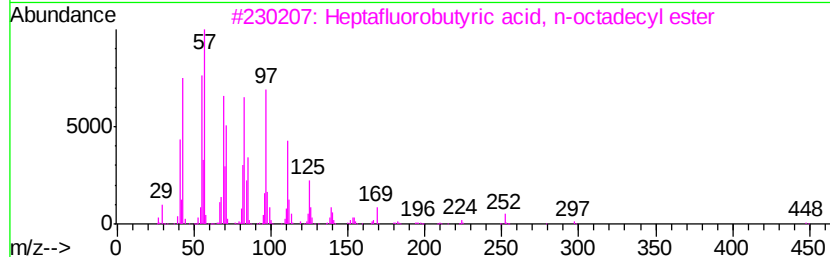
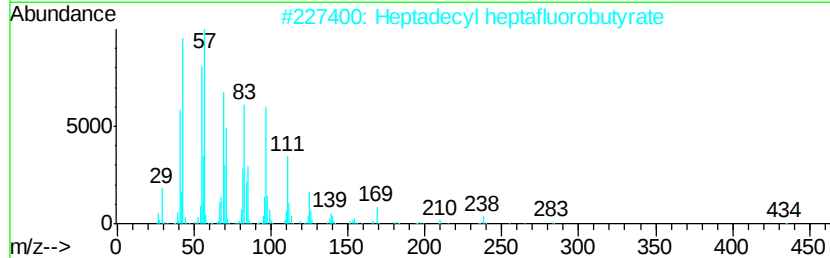
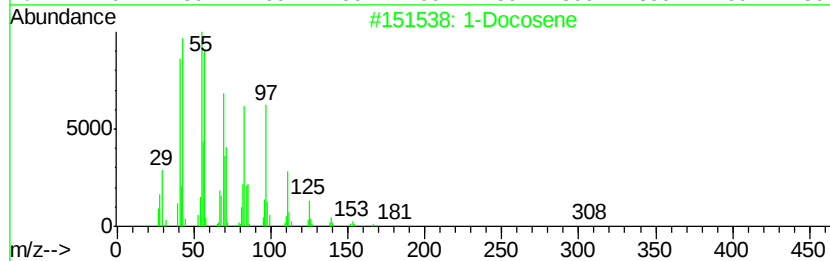
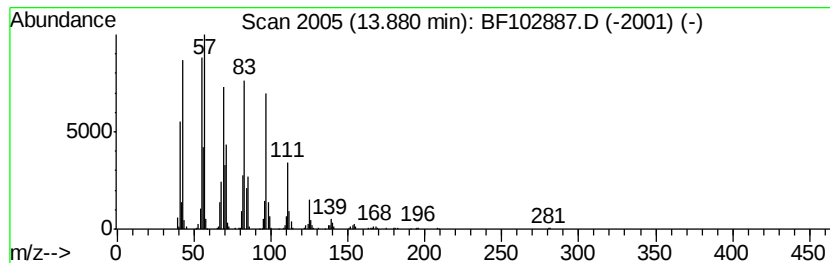
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	12.74 ng	631683	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	94
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3		Heptafluorobutvric acid, n-octadec...	466	C22H37F7O2	000400-57-7	91
4		Octacosanol	410	C28H58O	000557-61-9	91
5		2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020918\
Data File : BF102887.D
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Operator : SJ/JU
Sample : J1476-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

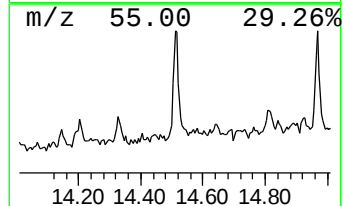
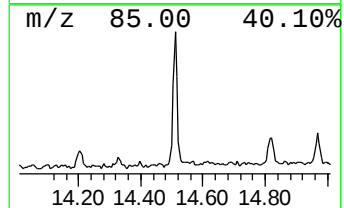
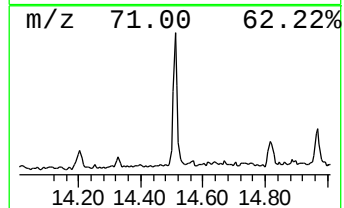
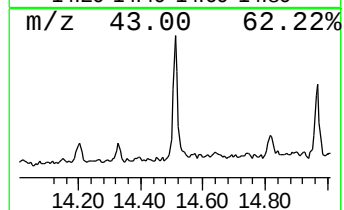
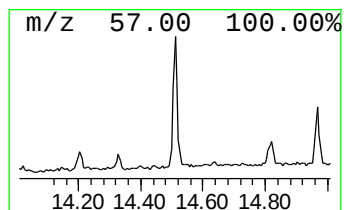
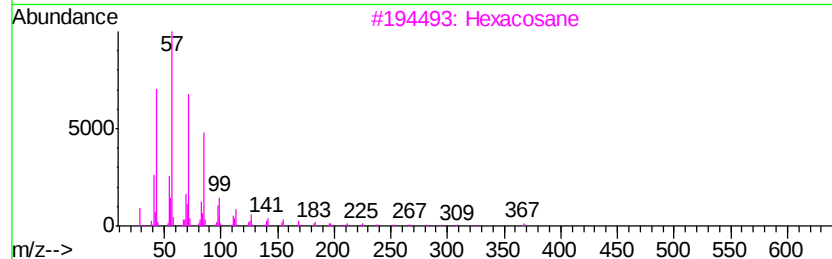
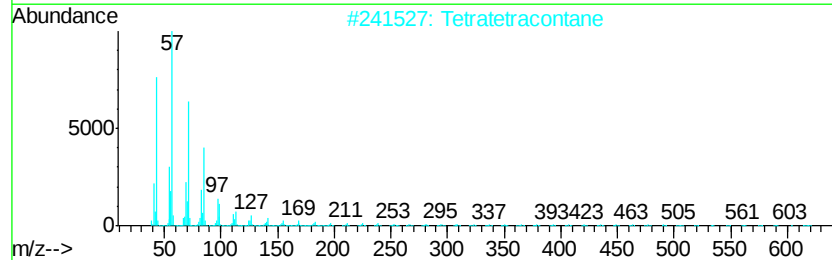
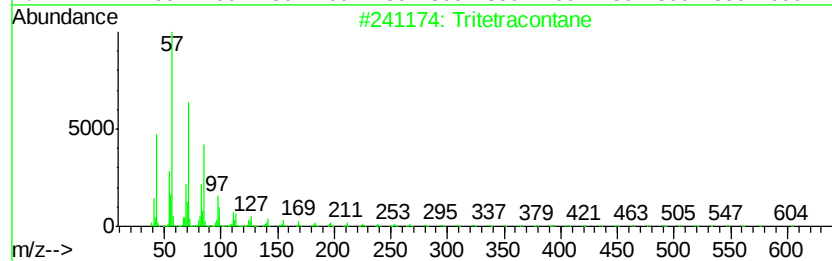
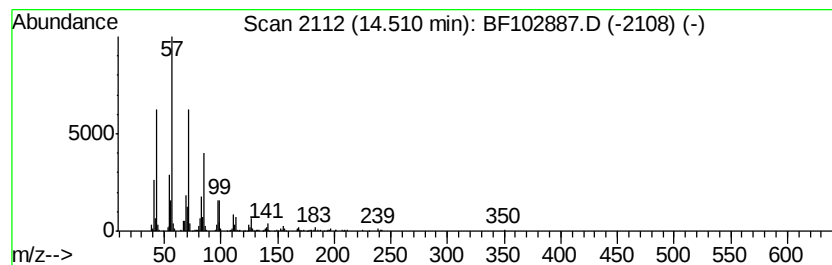
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tritetracontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.51	5.82 ng	288517	Chrysene-d12		14.05	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tritetracontane	605	C43H88	007098-21-7	91
2		Tetratetracontane	619	C44H90	007098-22-8	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020918\
Data File : BF102887.D
Acq On : 9 Feb 2018 14:33
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Misc :
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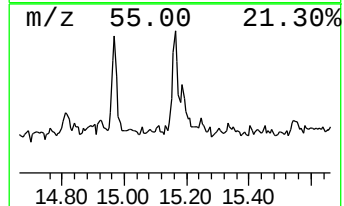
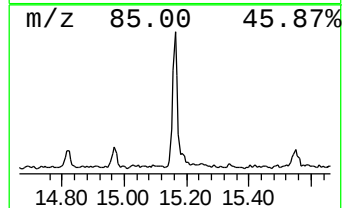
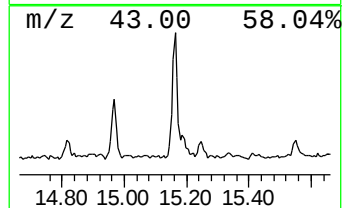
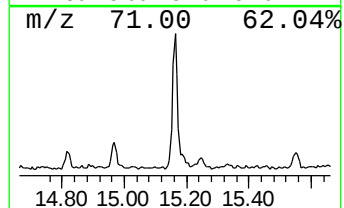
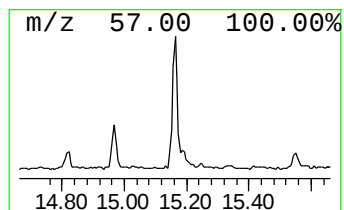
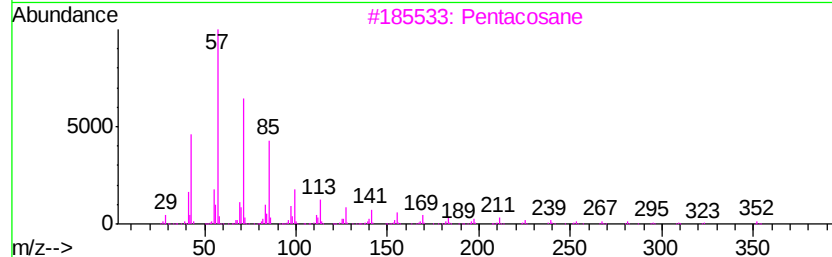
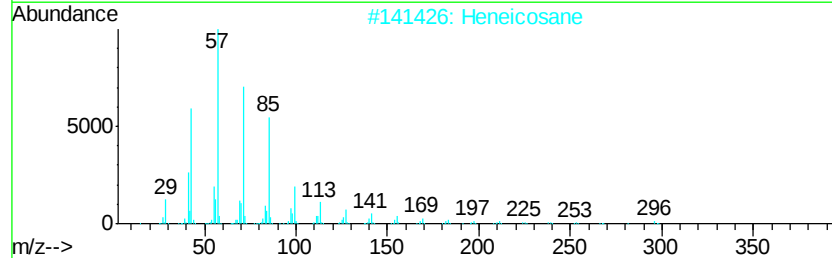
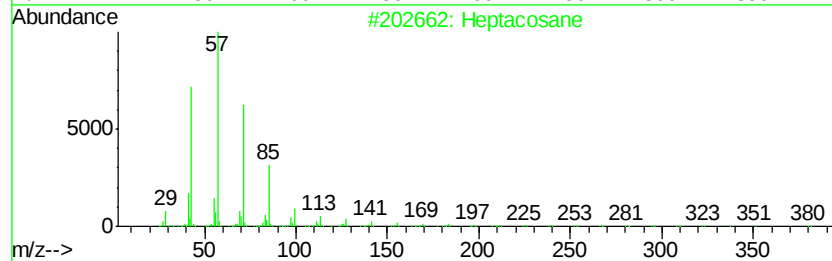
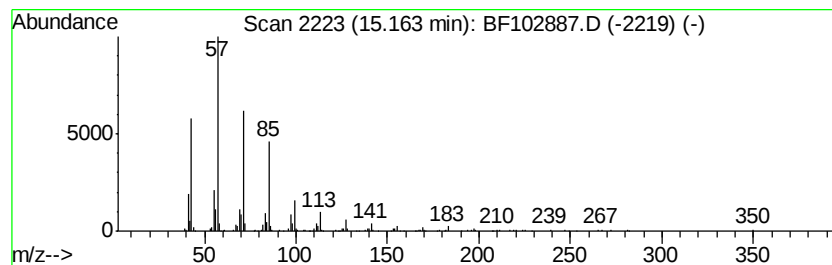
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	6.53 ng	319232	Perylene-d12	15.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Heneicosane		296	C21H44	000629-94-7	90
3	Pentacosane		352	C25H52	000629-99-2	90
4	Tridecane, 2-methyl-		198	C14H30	001560-96-9	87
5	Octadecane		254	C18H38	000593-45-3	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
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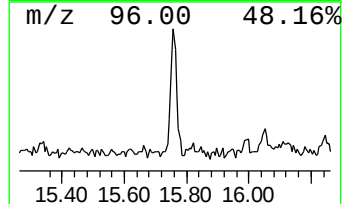
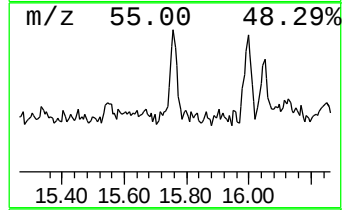
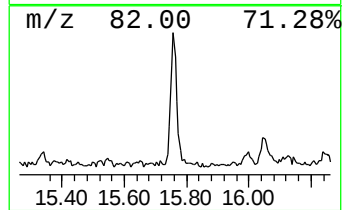
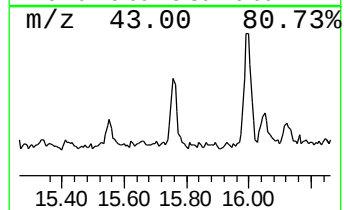
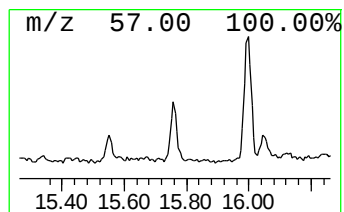
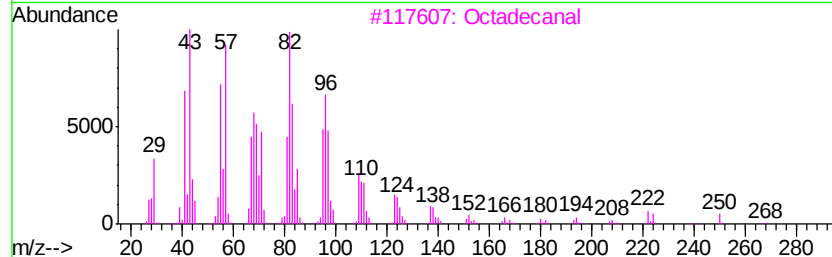
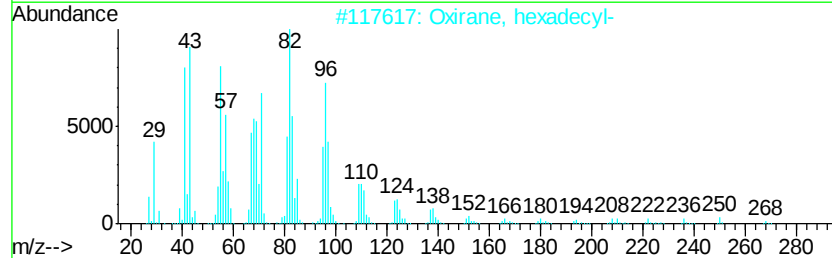
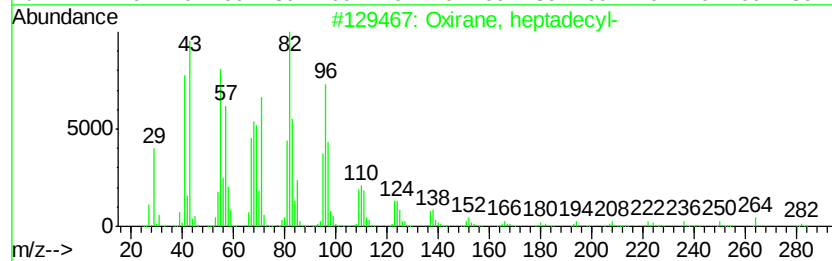
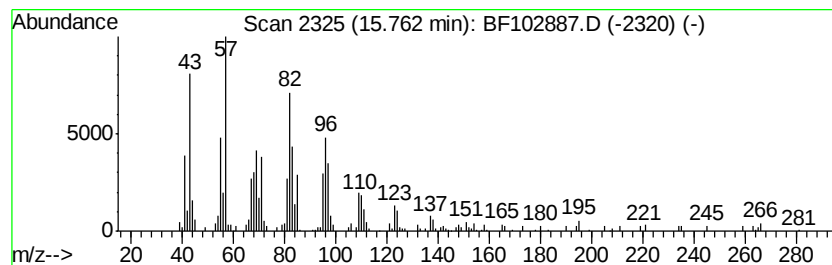
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Oxirane, heptadecyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.76	4.32 ng	211162	Perylene-d12	15.54	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3	Octadecanal	268	C18H36O	000638-66-4	87
4	Hexadecanal	240	C16H32O	000629-80-1	86
5	1,19-Eicosadiene	278	C20H38	014811-95-1	76



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
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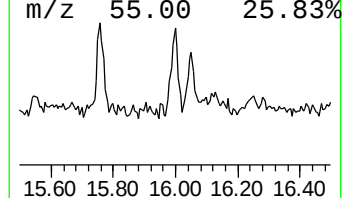
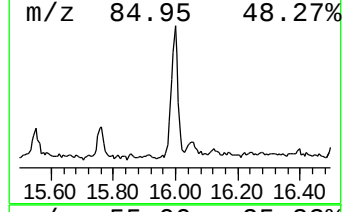
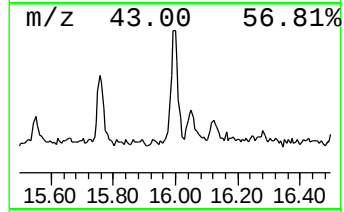
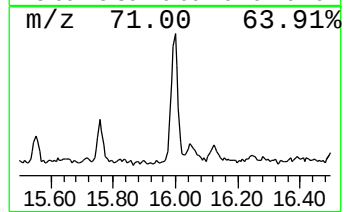
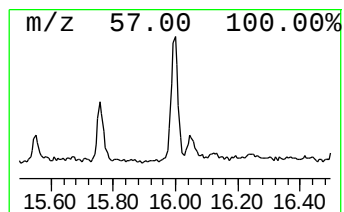
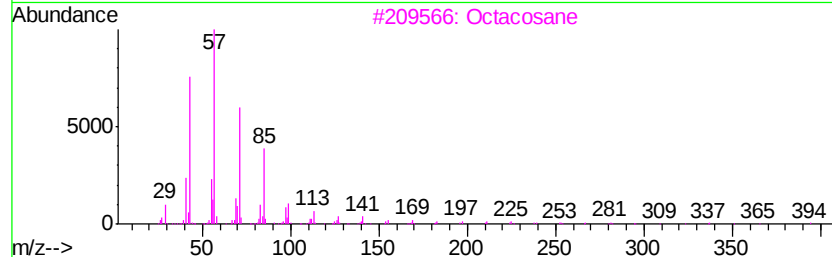
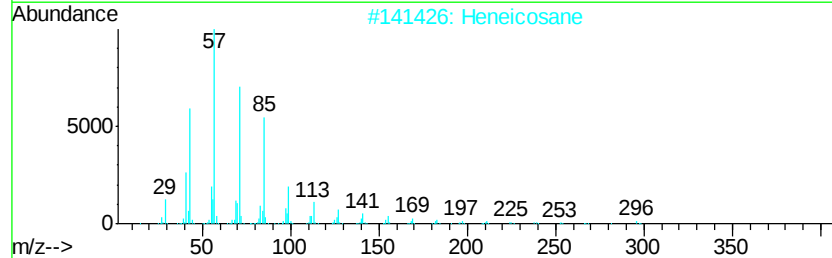
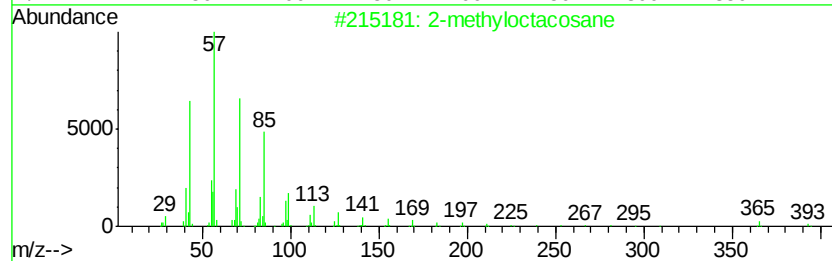
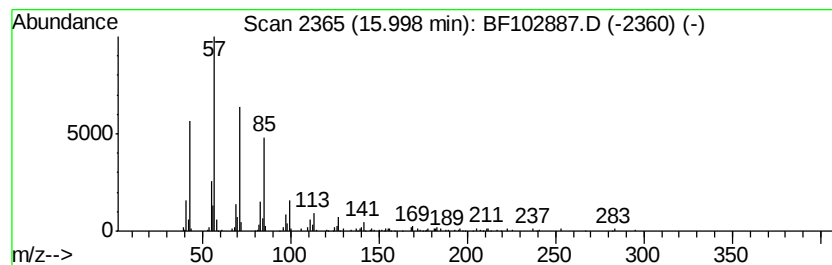
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	4.98 ng	243559	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Octacosane	394	C28H58	000630-02-4	87
4		Nonadecane	268	C19H40	000629-92-5	87
5		Octadecane	254	C18H38	000593-45-3	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020918\
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Acq On : 9 Feb 2018 14:33
Operator : SJ/JU
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Misc :
ALS Vial : 13 Sample Multiplier: 1

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ClientSampleId :
GL-WC-03

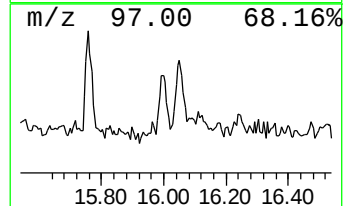
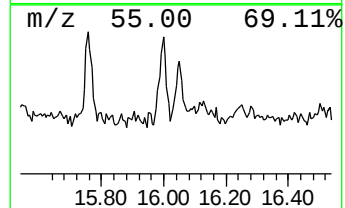
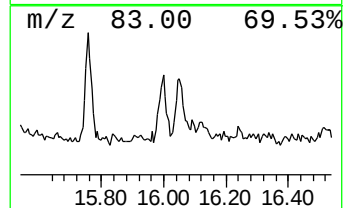
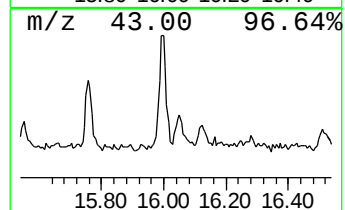
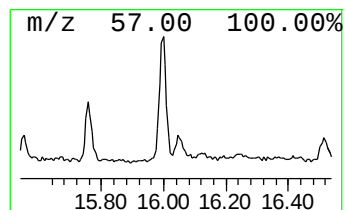
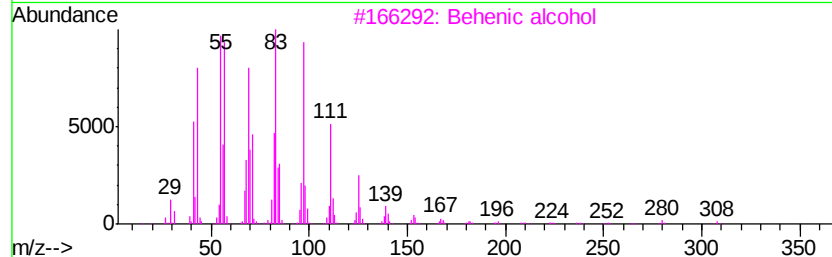
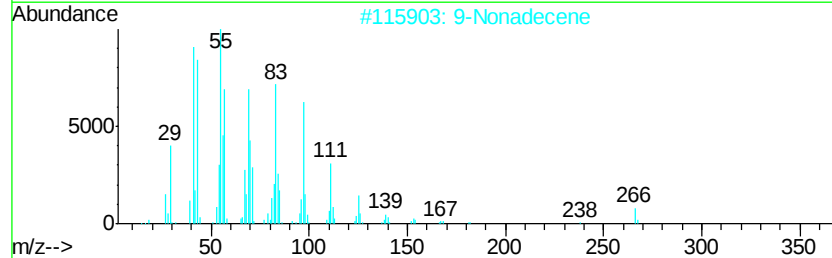
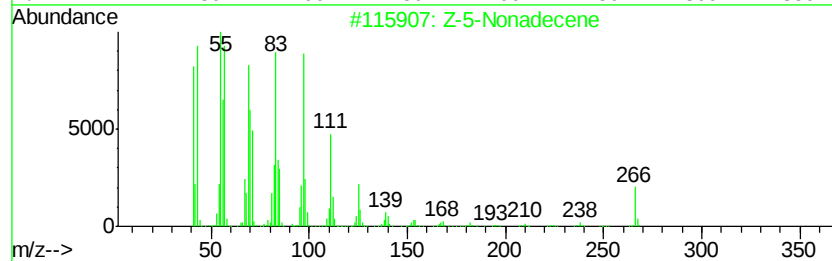
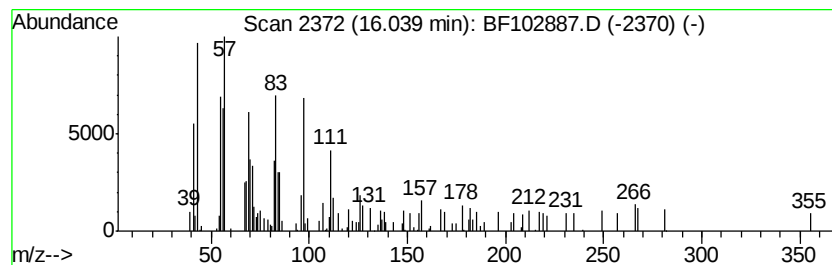
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Z-5-Nonadecene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.04	2.09 ng	102215	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Z-5-Nonadecene	266	C19H38	1000131-11-8	89
2		9-Nonadecene	266	C19H38	031035-07-1	86
3		Behenic alcohol	326	C22H46O	000661-19-8	83
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	70
5		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	70



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102887.D
Acq On : 9 Feb 2018 14:33
Operator : SJ/JU
Sample : J1476-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GL-WC-03

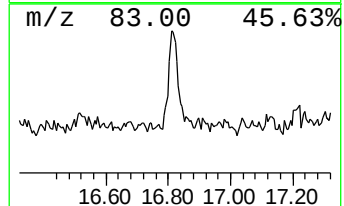
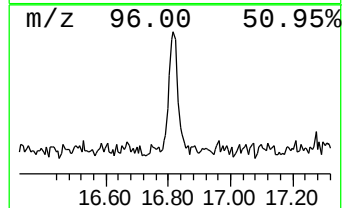
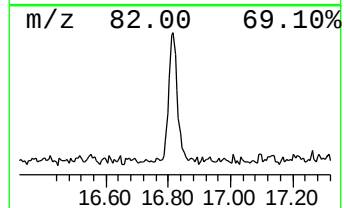
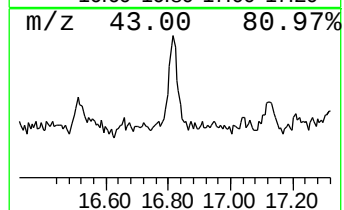
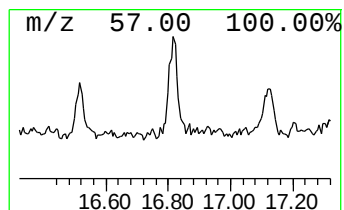
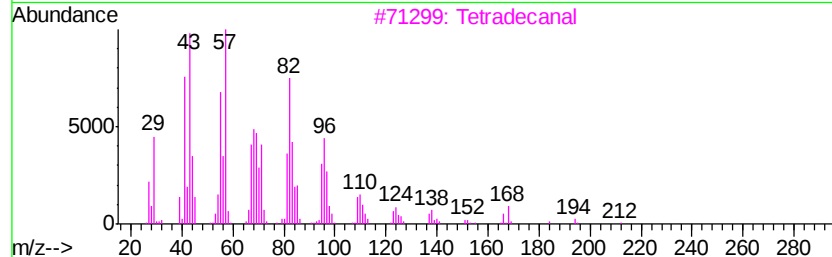
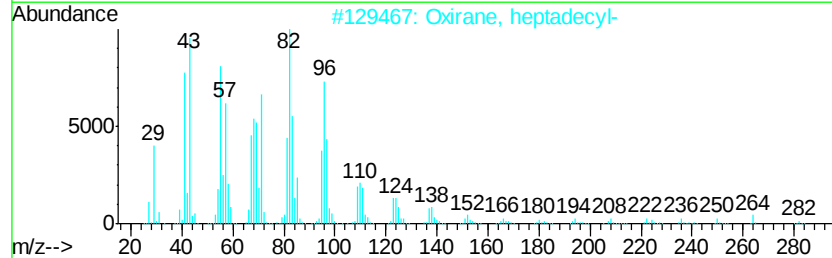
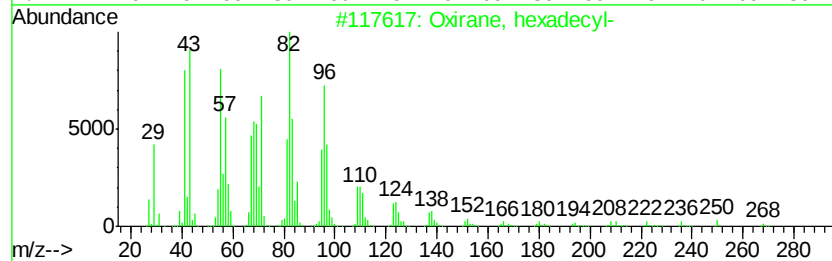
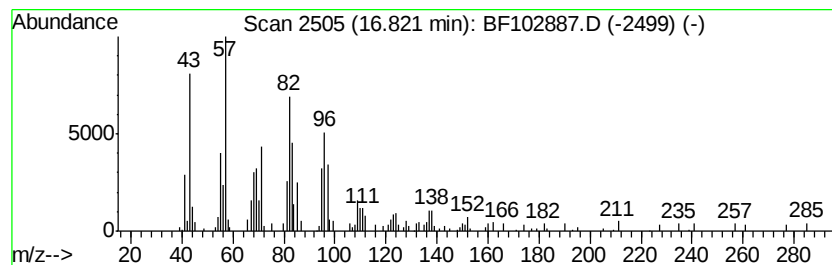
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Oxirane, hexadecyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.82	4.26 ng	208263	Perylene-d12	15.54

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	81
2			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	81
3			Tetradecanal	212	C14H28O	000124-25-4	80
4			Octadecanal	268	C18H36O	000638-66-4	72
5			Tridecanal	198	C13H26O	010486-19-8	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020918\
 Data File : BF102887.D
 Acq On : 9 Feb 2018 14:33
 Operator : SJ/JU
 Sample : J1476-05
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GL-WC-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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
Butane, 2-methoxy...	2.16	12.1	ng	614553	1	6.89	1019780	20.0
2-Pentanone, 4-hy...	5.12	79.4	ng	4050790	1	6.89	1019780	20.0
unknown6.65	6.65	51.3	ng	2615030	1	6.89	1019780	20.0
Hexadecane	9.85	2.1	ng	123548	3	9.92	1183610	20.0
Heptadecane	10.35	2.5	ng	147820	3	9.92	1183610	20.0
Tetratetracontane	10.82	3.4	ng	173656	4	11.41	1035320	20.0
1-Docosene	13.88	12.7	ng	631683	5	14.05	991438	20.0
Tritetracontane	14.51	5.8	ng	288517	5	14.05	991438	20.0
Heptacosane	15.16	6.5	ng	319232	6	15.54	978056	20.0
Oxirane, heptadecyl-	15.76	4.3	ng	211162	6	15.54	978056	20.0
2-methyloctacosane	16.00	5.0	ng	243559	6	15.54	978056	20.0
Z-5-Nonadecene	16.04	2.1	ng	102215	6	15.54	978056	20.0
Oxirane, hexadecyl-	16.82	4.3	ng	208263	6	15.54	978056	20.0