

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020618\
 Data File : BF102789.D
 Acq On : 6 Feb 2018 17:34
 Operator : SJ/JU
 Sample : J1454-20
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-03(6-WATER-LINE-BOTTEM@10

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	2.199	12	19	25	rVB	519135	689604	13.33%	1.533%
2	5.122	513	516	525	rVB	291439	380489	7.35%	0.846%
3	5.510	576	582	585	rBV	4633386	5175221	100.00%	11.503%
4	6.510	746	752	755	rBV	4391361	5105800	98.66%	11.349%
5	6.651	771	776	780	rBV	4633615	5050520	97.59%	11.226%
6	6.881	811	815	819	rVB	1451002	1255891	24.27%	2.791%
7	7.040	838	842	845	rBV	4226901	3943108	76.19%	8.764%
8	7.445	905	911	914	rBV	3174241	3250616	62.81%	7.225%
9	8.163	1029	1033	1037	rBV	1835874	1597423	30.87%	3.551%
10	9.239	1211	1216	1219	rBV	4902303	4907693	94.83%	10.908%
11	9.316	1225	1229	1231	rBV	111994	99122	1.92%	0.220%
12	9.628	1278	1282	1285	rBV	559796	496279	9.59%	1.103%
13	9.845	1316	1319	1322	rVB	262823	202959	3.92%	0.451%
14	9.922	1328	1332	1336	rBV	1676909	1491816	28.83%	3.316%
15	10.163	1370	1373	1378	rBV2	68485	84368	1.63%	0.188%
16	10.322	1397	1400	1401	rBV	84094	75518	1.46%	0.168%
17	10.345	1401	1404	1407	rVB	309486	231778	4.48%	0.515%
18	10.563	1436	1441	1444	rBV	148880	175871	3.40%	0.391%
19	10.710	1462	1466	1469	rBV	2383717	2122951	41.02%	4.719%
20	10.816	1481	1484	1490	rBV	274265	363780	7.03%	0.809%
21	11.263	1557	1560	1563	rBV	188263	163508	3.16%	0.363%
22	11.292	1563	1565	1572	rVB	171135	181877	3.51%	0.404%
23	11.404	1581	1584	1587	rBV	1223389	1179043	22.78%	2.621%
24	11.427	1587	1588	1594	rVB2	115196	112598	2.18%	0.250%
25	11.692	1630	1633	1636	rVV	139385	108292	2.09%	0.241%
26	11.927	1670	1673	1681	rBV3	147885	152896	2.95%	0.340%
27	12.098	1700	1702	1705	rBV	112749	86633	1.67%	0.193%
28	12.380	1747	1750	1752	rBV	60749	51927	1.00%	0.115%
29	12.486	1766	1768	1772	rBV	57649	53966	1.04%	0.120%
30	12.616	1788	1790	1795	rVB	165209	153689	2.97%	0.342%
31	12.851	1824	1830	1833	rBV2	157259	222045	4.29%	0.494%
32	12.992	1850	1854	1857	rBV	3113540	2840853	54.89%	6.314%
33	13.874	2001	2004	2008	rBV	681007	643670	12.44%	1.431%
34	14.045	2029	2033	2036	rBV	1065636	1055226	20.39%	2.345%

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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

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35	14.798	2159	2161	2167	rBV	219907	250856	4.85%	0.558%
36	15.527	2281	2285	2296	rVB	735733	1032578	19.95%	2.295%

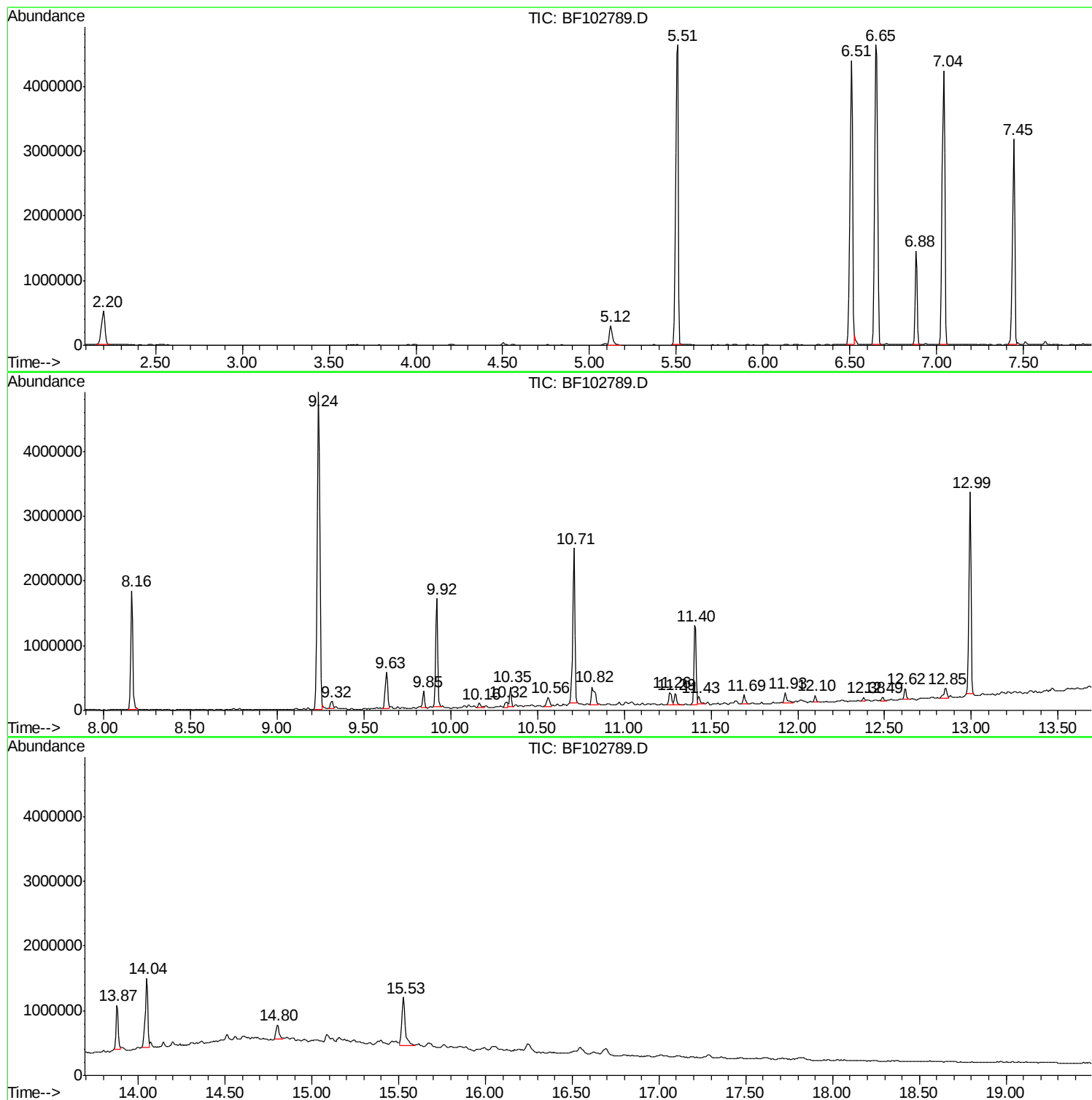
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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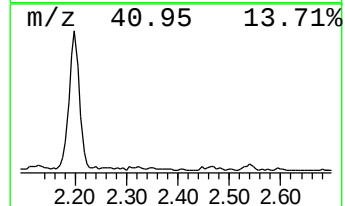
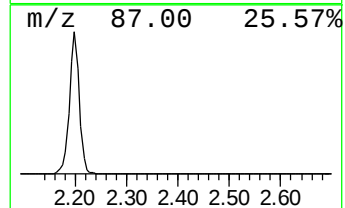
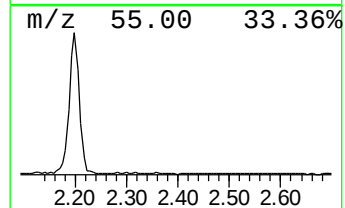
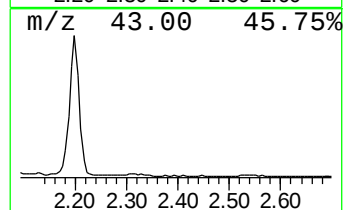
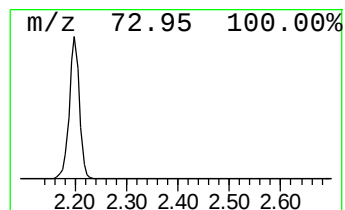
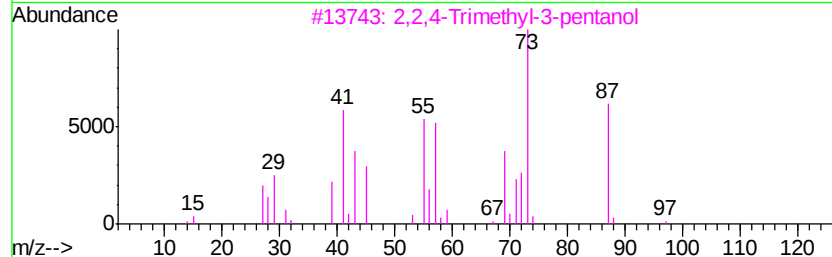
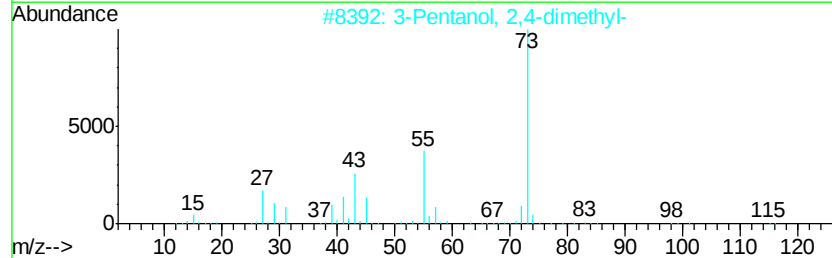
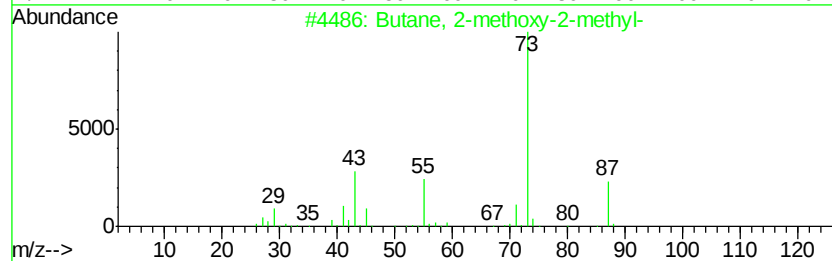
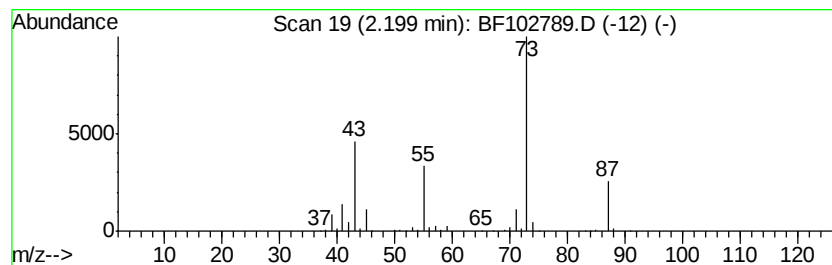
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	10.98 ng	689604	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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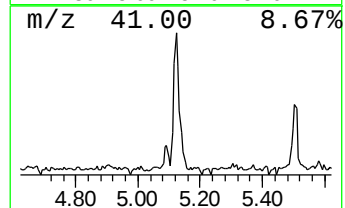
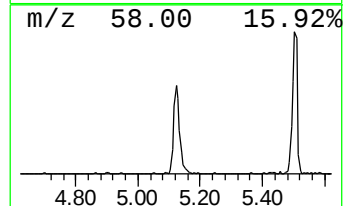
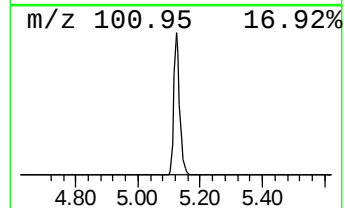
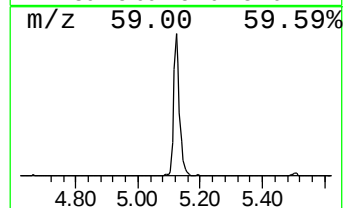
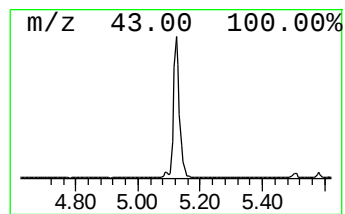
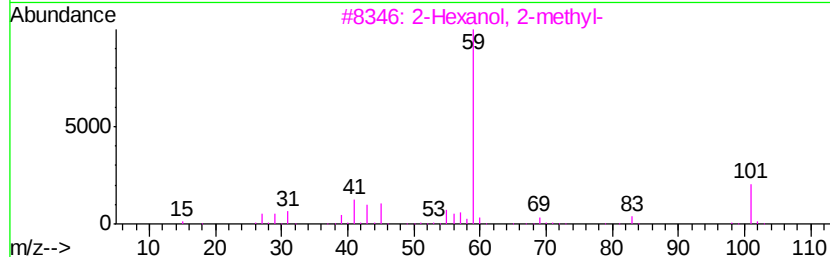
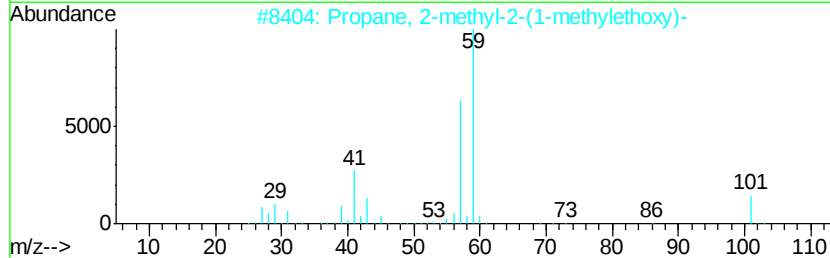
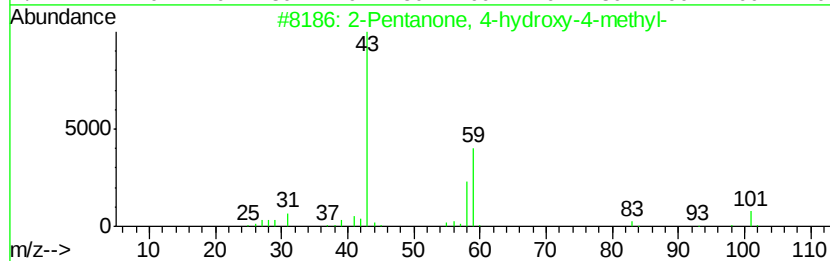
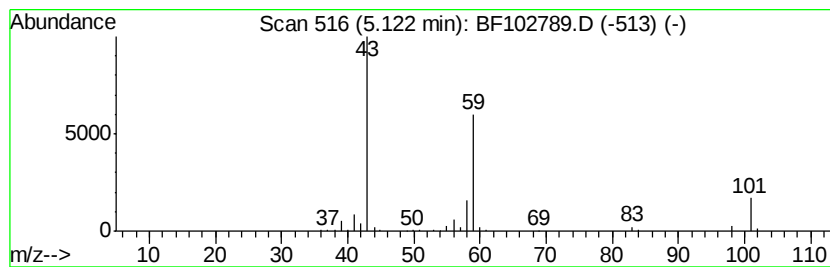
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	6.06 ng	380489	1,4-Dichlorobenzene-d4	6.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
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			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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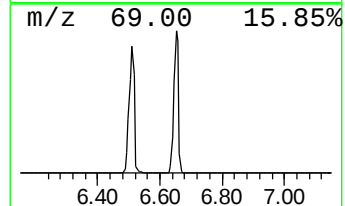
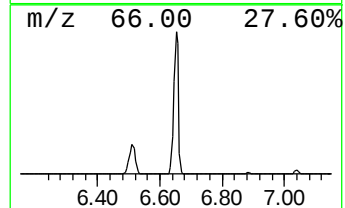
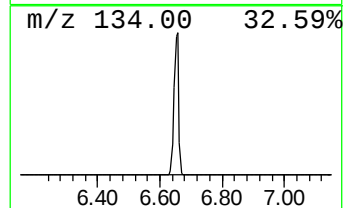
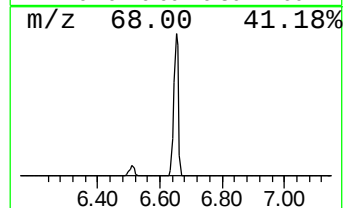
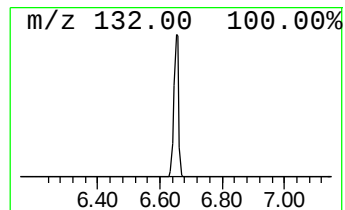
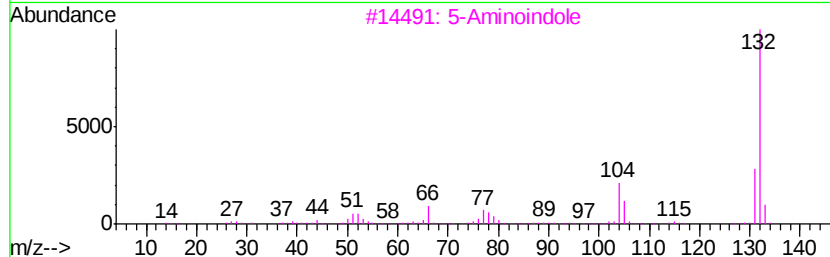
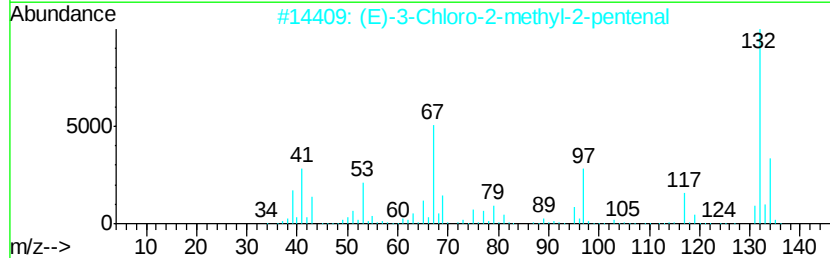
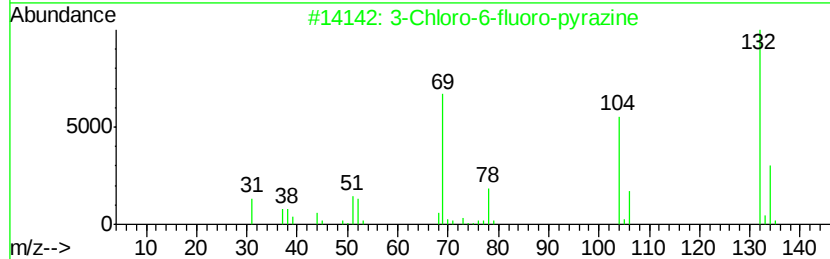
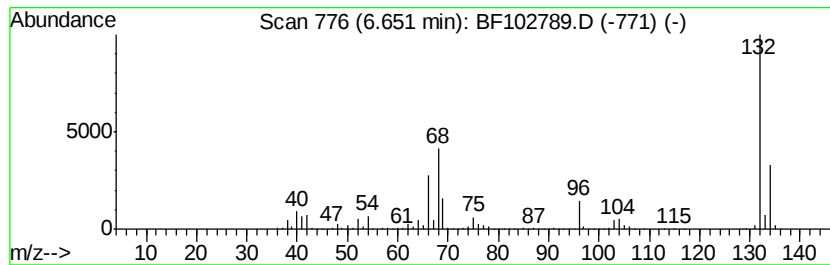
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	80.43 ng	5050520	1,4-Dichlorobenzene-d4	6.88

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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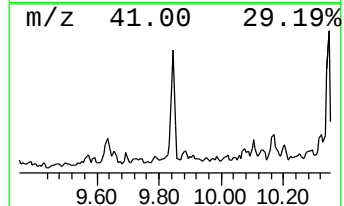
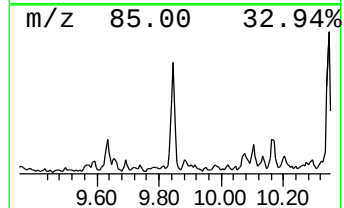
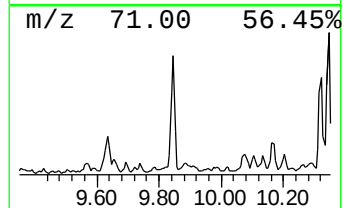
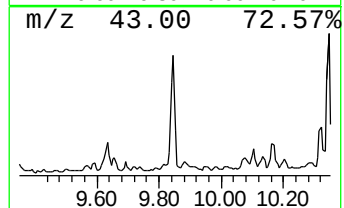
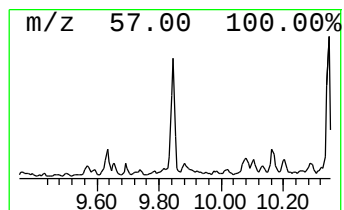
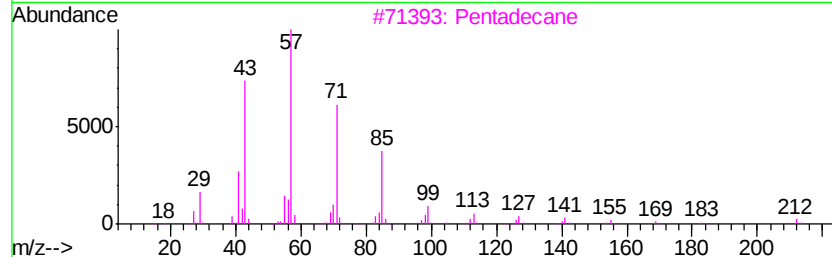
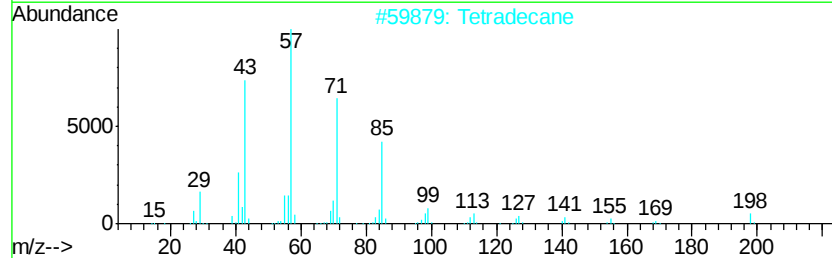
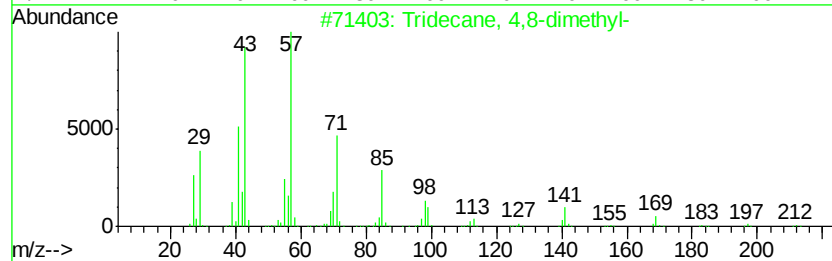
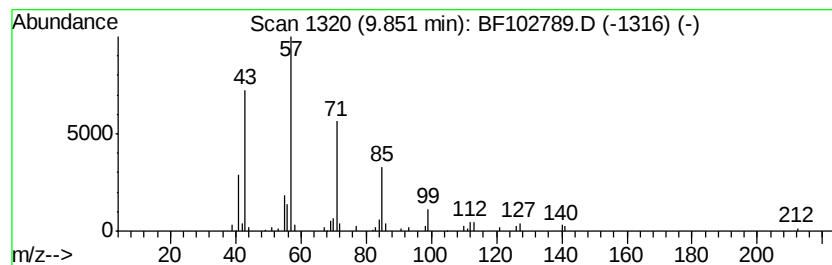
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Tridecane, 4,8-dimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
9.85	2.72 ng	202959	Acenaphthene-d10		9.92
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 4,8-dimethyl-	212	C15H32	055030-62-1	90
2	Tetradecane	198	C14H30	000629-59-4	90
3	Pentadecane	212	C15H32	000629-62-9	87
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	80
5	Hexadecane	226	C16H34	000544-76-3	80



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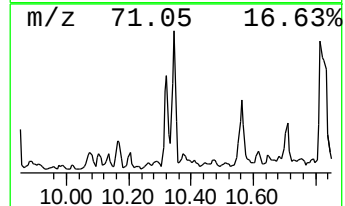
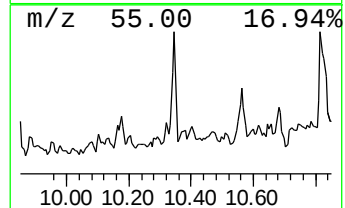
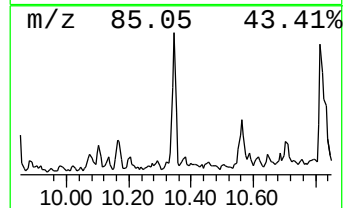
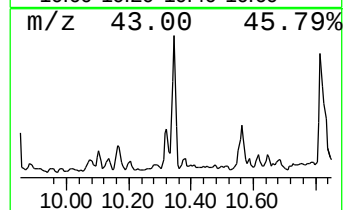
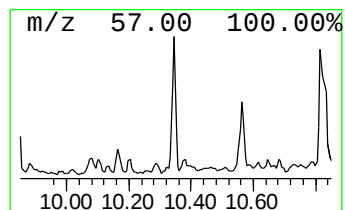
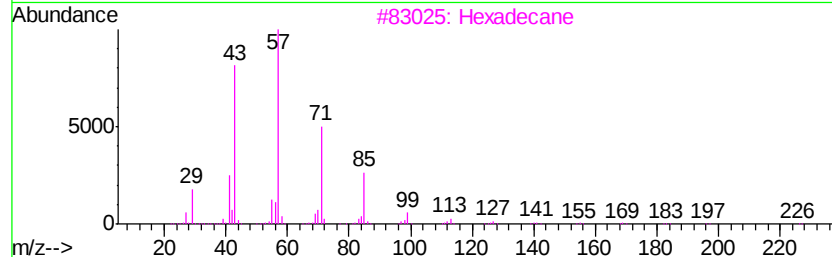
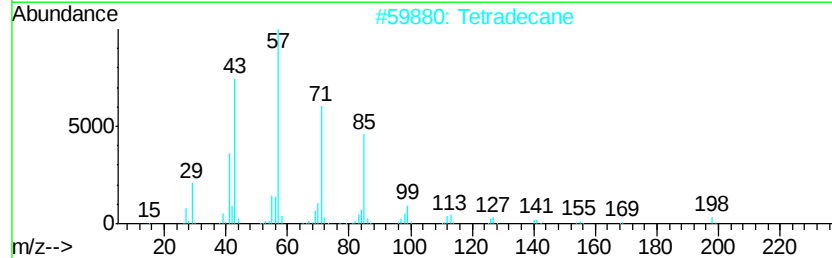
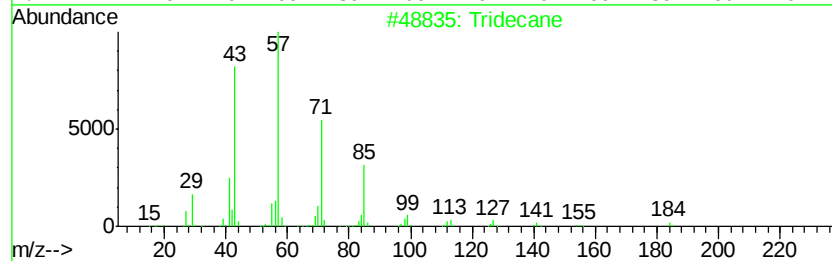
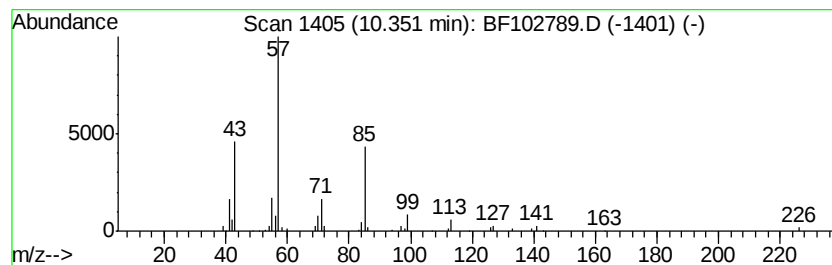
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Peak Number 6 Tridecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.35	3.11 ng	231778	Acenaphthene-d10		9.92
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Tetradecane	198	C14H30	000629-59-4	86
3	Hexadecane	226	C16H34	000544-76-3	86
4	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	80
5	Pentadecane	212	C15H32	000629-62-9	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020618\
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Acq On : 6 Feb 2018 17:34
Operator : SJ/JU
Sample : J1454-20
Misc :
ALS Vial : 19 Sample Multiplier: 1

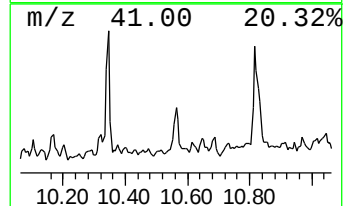
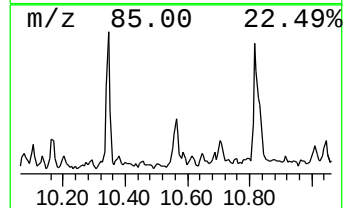
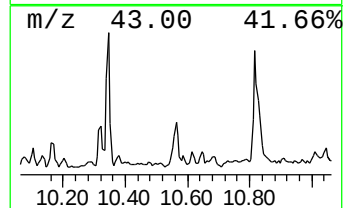
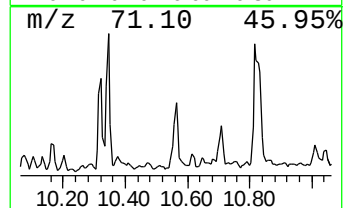
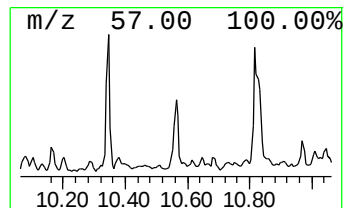
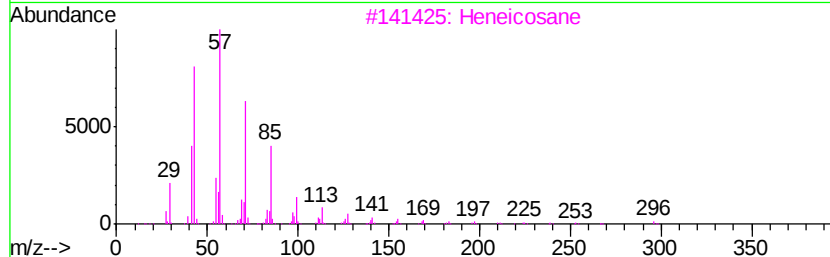
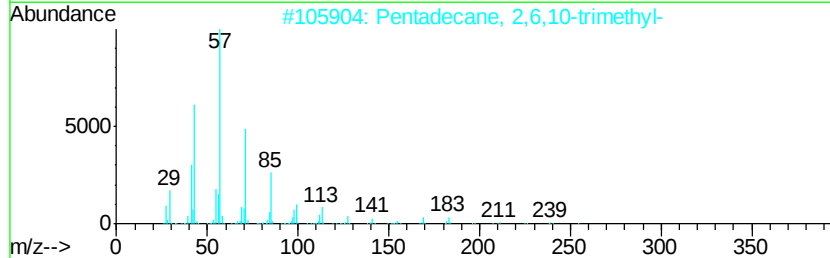
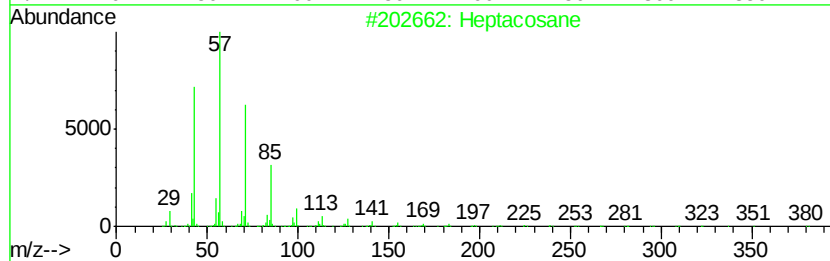
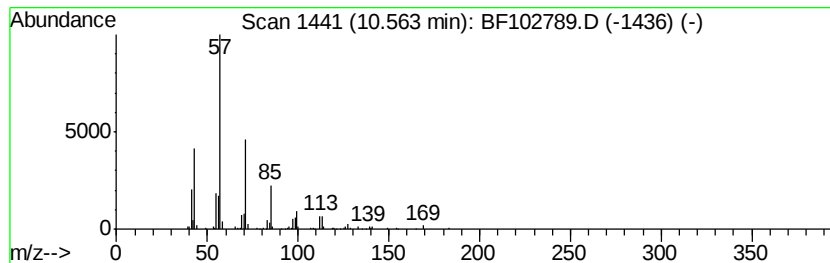
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ClientSampleId :
TP-03(6-WATER-LINE-BOTTEM@10

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 7 Heptacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.56	2.36 ng	175871	Acenaphthene-d10	9.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptacosane	380 C27H56	000593-49-7	87
2	Pentadecane, 2,6,10-trimethyl-	254 C18H38	003892-00-0	78
3	Heneicosane	296 C21H44	000629-94-7	64
4	Hexadecane	226 C16H34	000544-76-3	64
5	Undecane, 3,9-dimethyl-	184 C13H28	017301-31-4	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020618\
Data File : BF102789.D
Acq On : 6 Feb 2018 17:34
Operator : SJ/JU
Sample : J1454-20
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Instrument :
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ClientSampleId :
TP-03(6-WATER-LINE-BOTTEM@10

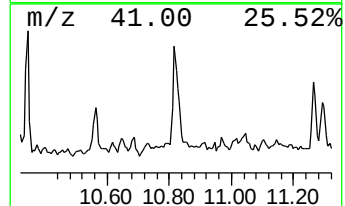
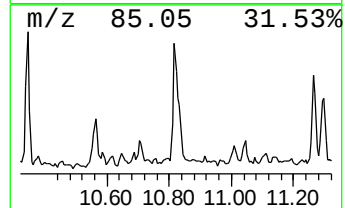
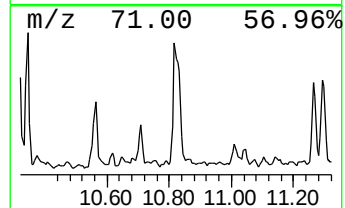
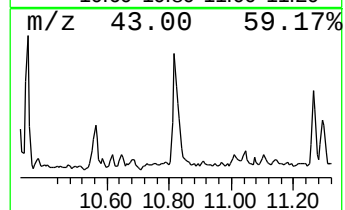
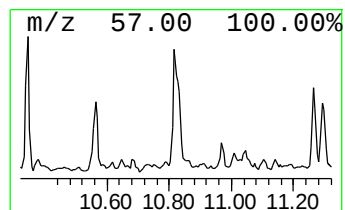
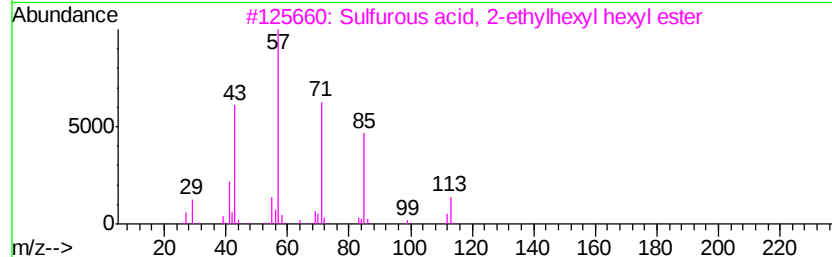
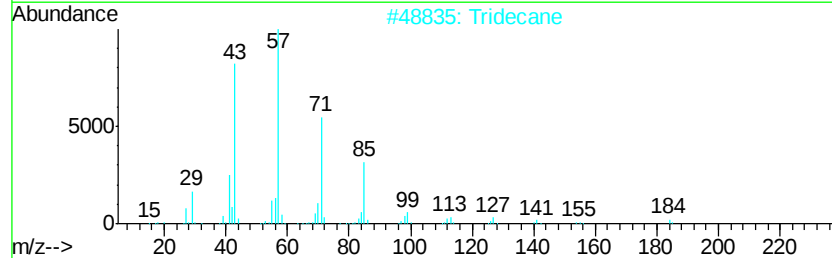
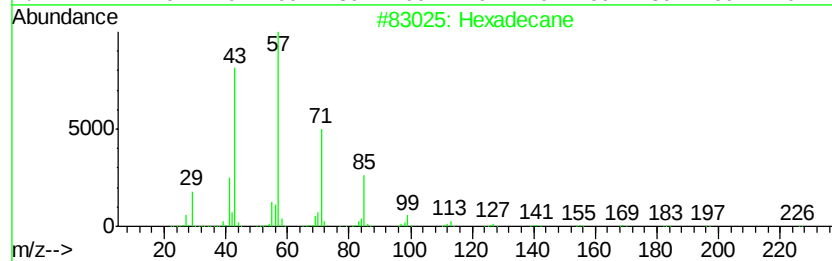
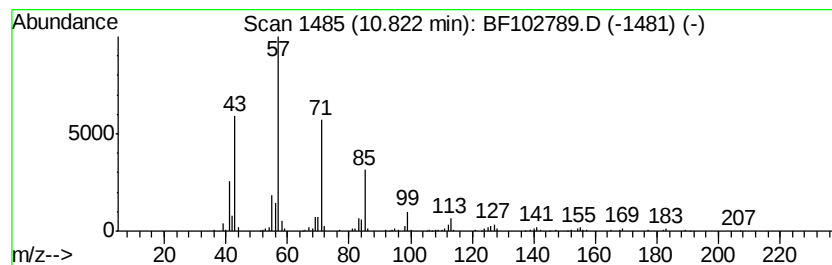
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	6.17 ng	363780	Phenanthrene-d10	11.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	90
2	Tridecane		184	C13H28	000629-50-5	83
3	Sulfurous acid, 2-ethylhexyl hex...		278	C14H30O3S	1000309-20-2	80
4	Octane, 3,5-dimethyl-		142	C10H22	015869-93-9	72
5	Dodecane, 2-methyl-6-propyl-		226	C16H34	055045-08-4	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020618\
Data File : BF102789.D
Acq On : 6 Feb 2018 17:34
Operator : SJ/JU
Sample : J1454-20
Misc :
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Instrument :
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ClientSampleId :
TP-03(6-WATER-LINE-BOTTEM@10)

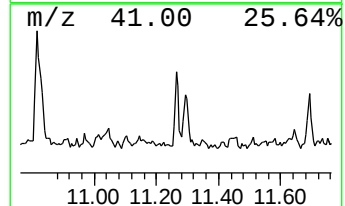
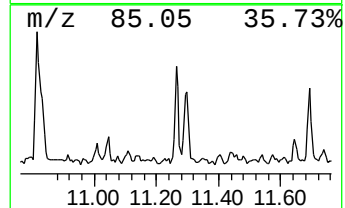
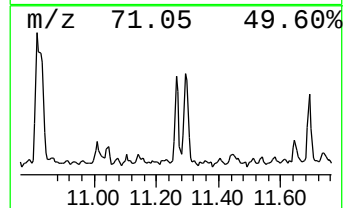
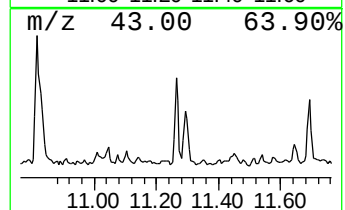
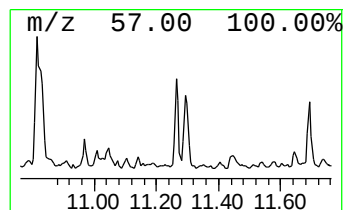
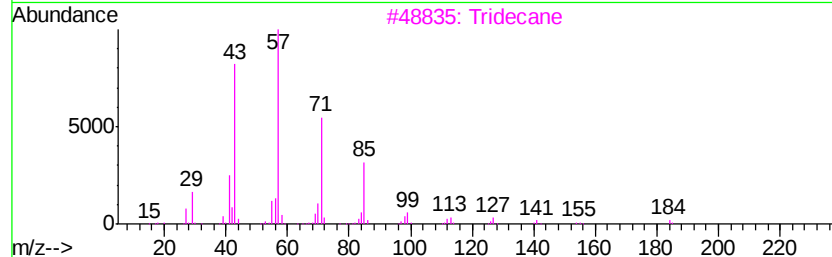
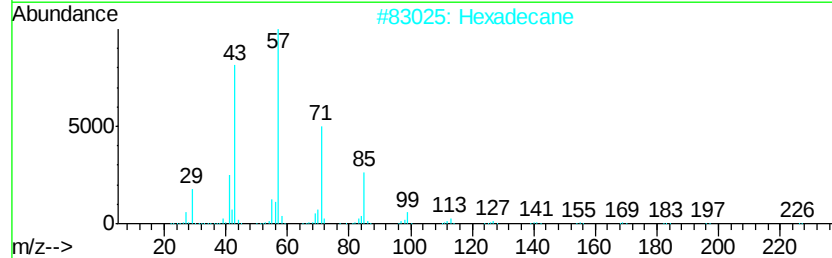
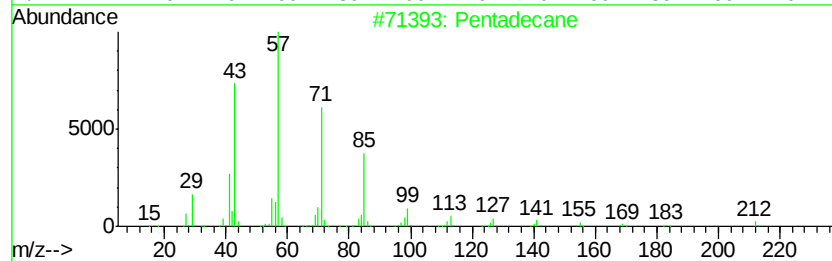
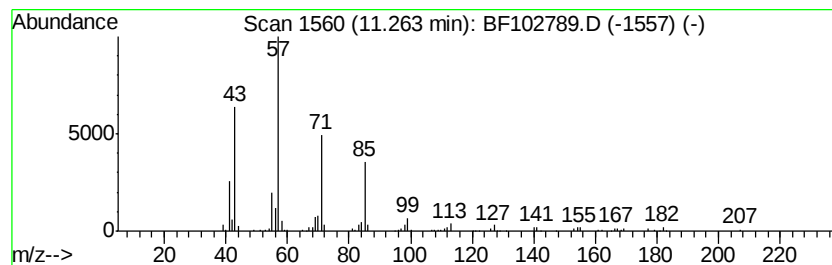
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.26	2.77 ng	163508	Phenanthrene-d10	11.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane		212	C15H32	000629-62-9	91
2	Hexadecane		226	C16H34	000544-76-3	90
3	Tridecane		184	C13H28	000629-50-5	86
4	Tritetracontane		605	C43H88	007098-21-7	83
5	Tetradecane		198	C14H30	000629-59-4	80



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020618\
Data File : BF102789.D
Acq On : 6 Feb 2018 17:34
Operator : SJ/JU
Sample : J1454-20
Misc :
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ClientSampleId :
TP-03(6-WATER-LINE-BOTTEM@10

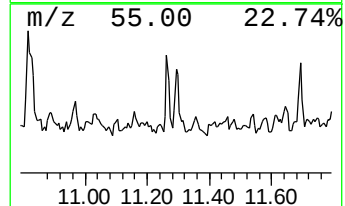
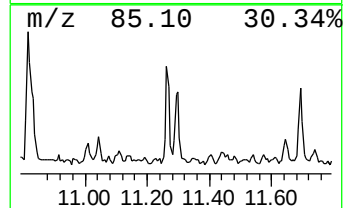
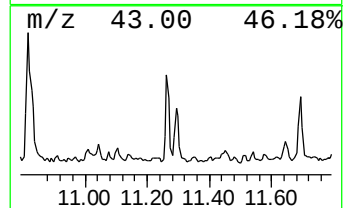
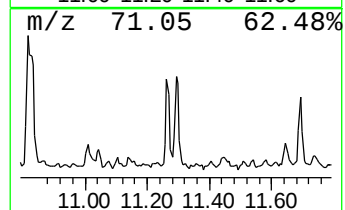
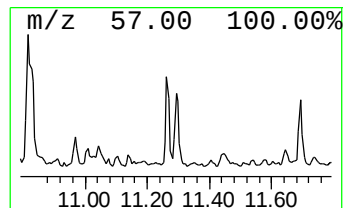
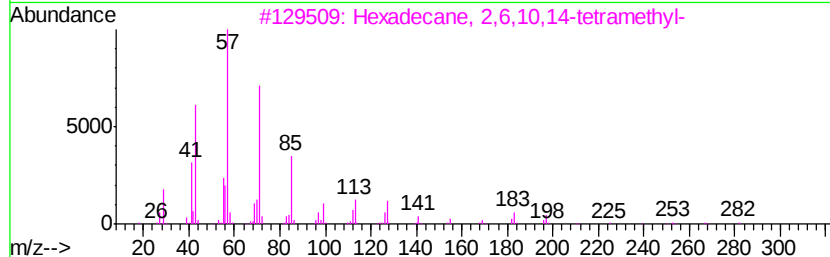
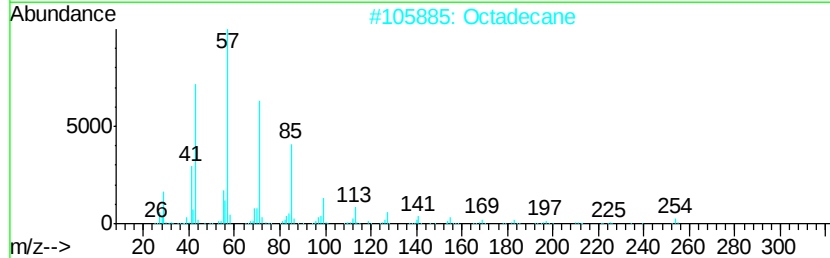
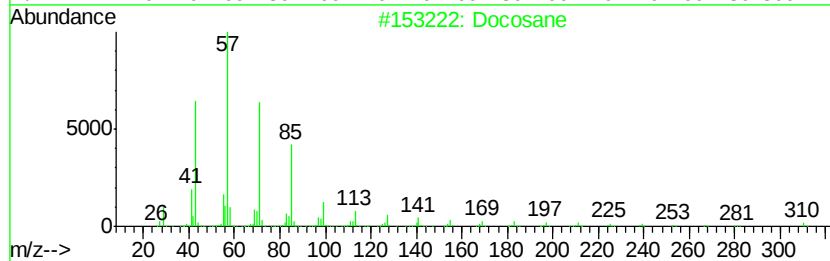
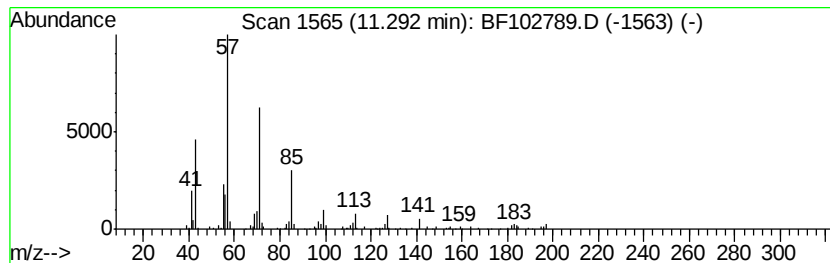
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Docosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.29	3.09 ng	181877	Phenanthrene-d10	11.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane	310	C22H46	000629-97-0	86
2		Octadecane	254	C18H38	000593-45-3	86
3		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	83
4		2-Bromo dodecane	248	C12H25Br	013187-99-0	72
5		Hexadecane	226	C16H34	000544-76-3	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020618\
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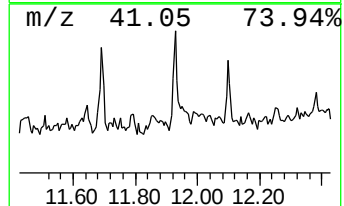
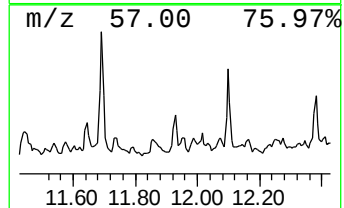
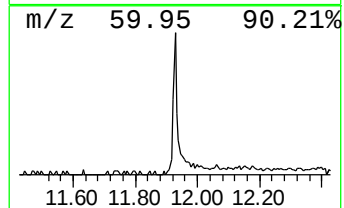
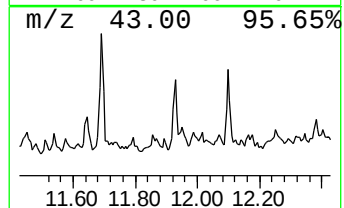
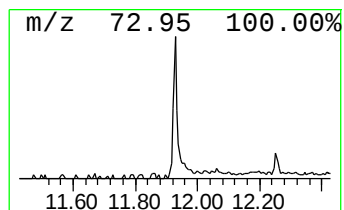
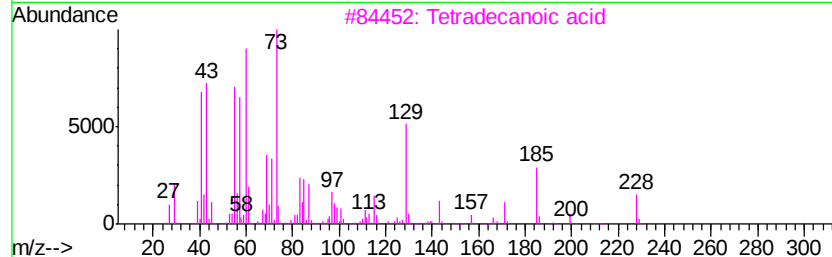
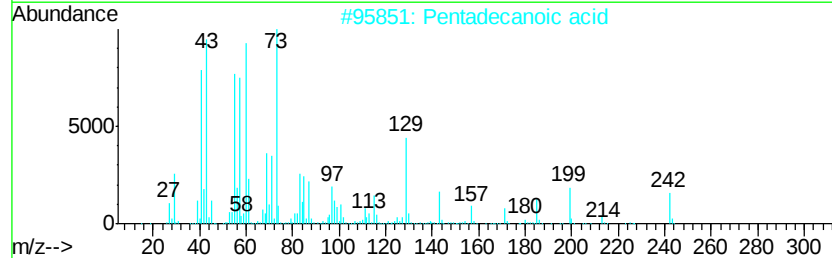
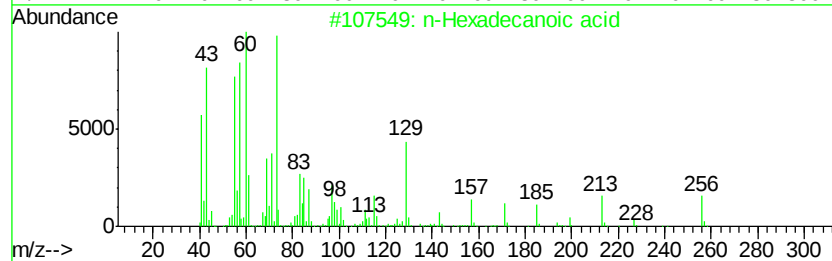
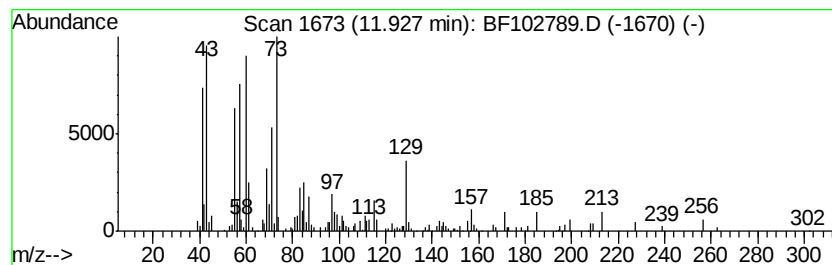
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TP-03(6-WATER-LINE-BOTTEM@10

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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 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.93	2.59 ng	152896	Phenanthrene-d10		11.40
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020618\
Data File : BF102789.D
Acq On : 6 Feb 2018 17:34
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TP-03(6-WATER-LINE-BOTTEM@10

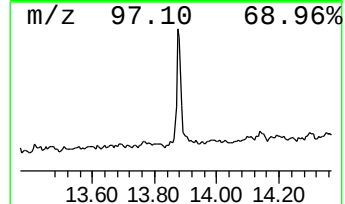
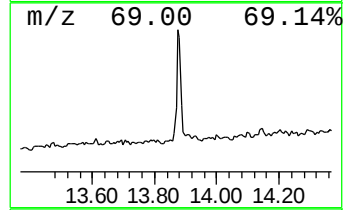
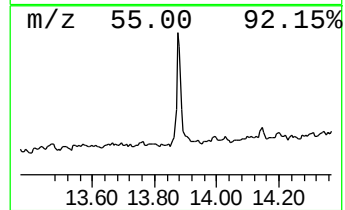
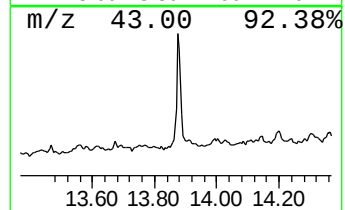
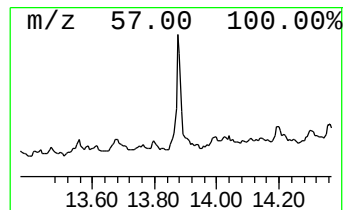
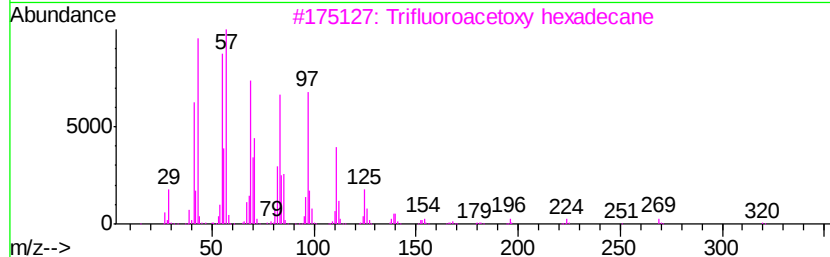
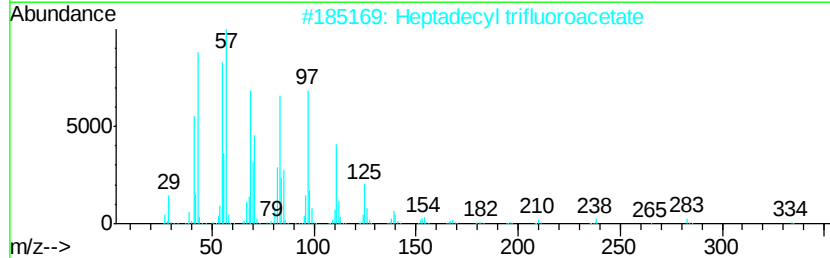
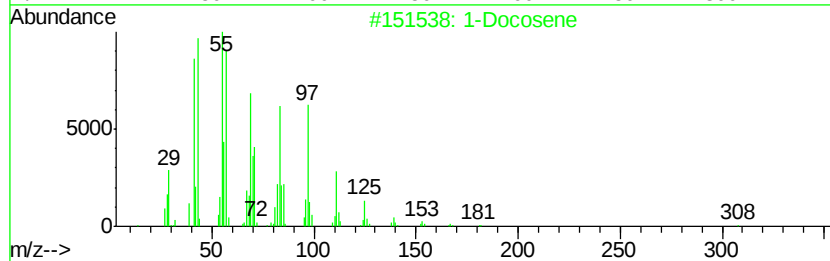
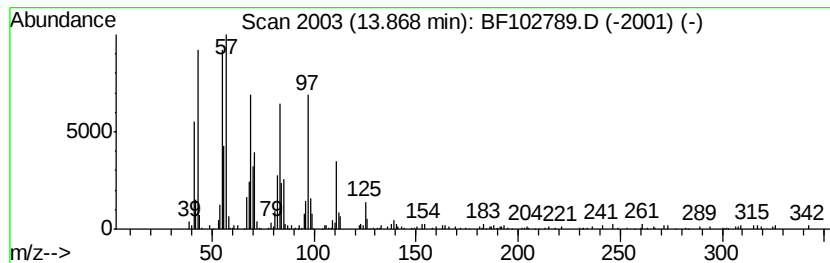
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	12.20 ng	643670	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	97
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
3		Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	91
4		1-Nonadecene	266	C19H38	018435-45-5	91
5		1-Octadecanol	270	C18H38O	000112-92-5	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020618\
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ClientSampleId :
TP-03(6-WATER-LINE-BOTTEM@10

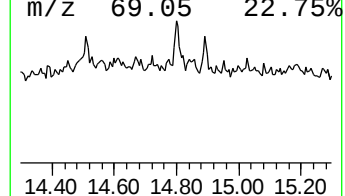
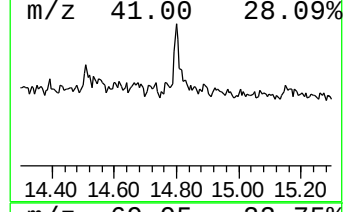
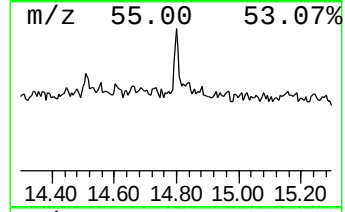
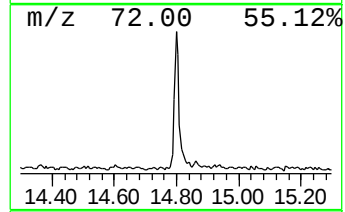
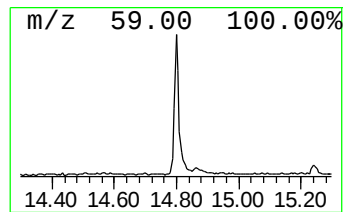
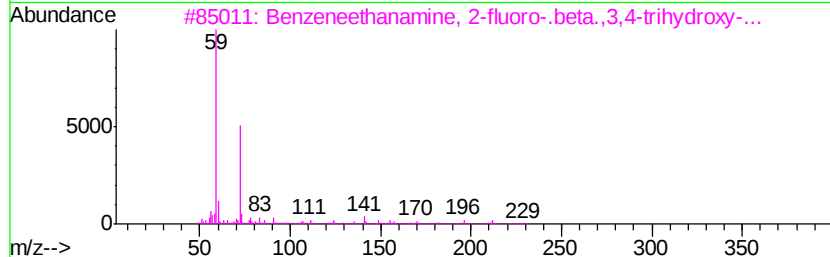
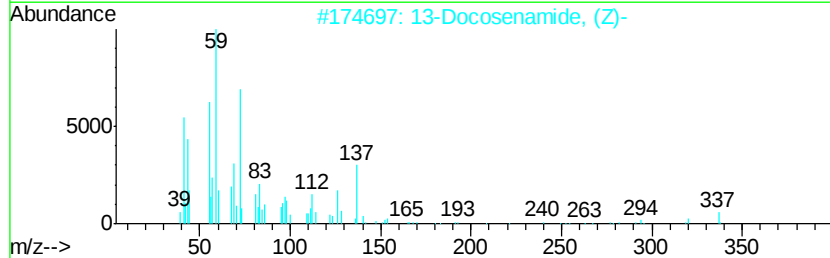
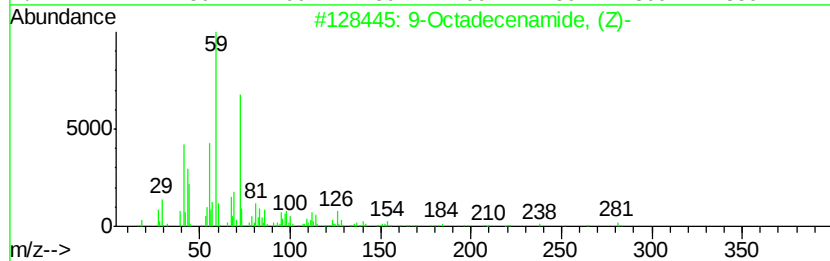
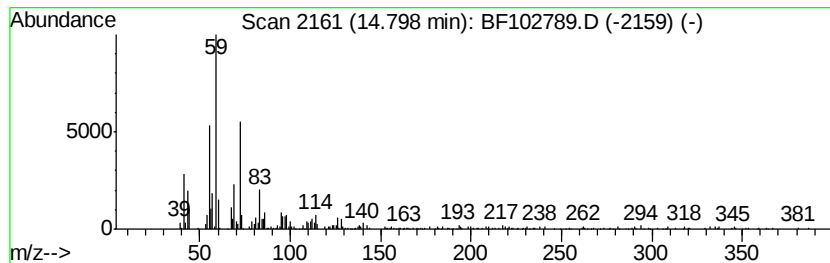
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	4.86 ng	250856	Perylene-d12	15.53

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	87
3			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59
4			Nonanamide	157	C9H19NO	001120-07-6	43
5			2-Hydroxy-2,4-dimethyl-hept-6-en...	156	C9H16O2	1000192-56-0	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020618\
 Data File : BF102789.D
 Acq On : 6 Feb 2018 17:34
 Operator : SJ/JU
 Sample : J1454-20
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-03(6-WATER-LINE-BOTTEM@10

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...	2.20	11.0	ng	689604	1	6.88	1255890	20.0
2-Pentanone, 4-hy...	5.12	6.1	ng	380489	1	6.88	1255890	20.0
unknown6.65	6.65	80.4	ng	5050520	1	6.88	1255890	20.0
Tridecane, 4,8-di...	9.85	2.7	ng	202959	3	9.92	1491820	20.0
Tridecane	10.35	3.1	ng	231778	3	9.92	1491820	20.0
Heptacosane	10.56	2.4	ng	175871	3	9.92	1491820	20.0
Hexadecane	10.82	6.2	ng	363780	4	11.40	1179040	20.0
Pentadecane	11.26	2.8	ng	163508	4	11.40	1179040	20.0
Docosane	11.29	3.1	ng	181877	4	11.40	1179040	20.0
n-Hexadecanoic acid	11.93	2.6	ng	152896	4	11.40	1179040	20.0
1-Docosene	13.87	12.2	ng	643670	5	14.05	1055230	20.0
9-Octadecenamide, ...	14.80	4.9	ng	250856	6	15.53	1032580	20.0