

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032717\
 Data File : BF093954.D
 Acq On : 27 Mar 2017 20:55
 Operator : SJ/MA
 Sample : I2405-02
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FRACTANK2

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-BF032217.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	4.075	368	372	378	rVB	201190	227035	4.05%	0.533%
2	4.463	434	438	442	rVB	2272617	2244868	40.09%	5.270%
3	5.169	554	558	564	rBV	110027	104602	1.87%	0.246%
4	5.528	614	619	622	rBV	1595405	1473070	26.31%	3.458%
5	5.681	639	645	648	rBV	3689359	3977895	71.05%	9.338%
6	5.934	684	688	692	rBV	967221	985617	17.60%	2.314%
7	6.116	714	719	723	rVB	3313858	3618743	64.63%	8.495%
8	6.587	792	799	802	rBV	2502768	3148645	56.24%	7.391%
9	6.775	812	831	833	rBV	303679	874340	15.62%	2.052%
10	6.910	850	854	860	rVB2	61846	73674	1.32%	0.173%
11	7.439	938	944	948	rBV	1341144	1362833	24.34%	3.199%
12	7.710	984	990	995	rVB2	59902	88064	1.57%	0.207%
13	7.775	995	1001	1011	rVB6	32190	78255	1.40%	0.184%
14	7.910	1014	1024	1029	rBV3	78517	174917	3.12%	0.411%
15	8.292	1083	1089	1100	rBV2	126538	151016	2.70%	0.354%
16	8.769	1162	1170	1173	rBV	4566074	5598922	100.00%	13.143%
17	8.980	1201	1206	1213	rVB	248391	244292	4.36%	0.573%
18	9.475	1287	1290	1301	rVB3	65661	144368	2.58%	0.339%
19	9.586	1301	1309	1313	rVV	1409524	1528715	27.30%	3.588%
20	9.627	1313	1316	1319	rVB	60775	56576	1.01%	0.133%
21	10.563	1466	1475	1478	rBV	2677990	3284874	58.67%	7.711%
22	10.698	1491	1498	1505	rBV	699117	705567	12.60%	1.656%
23	11.410	1613	1619	1623	rBV	1567418	1515260	27.06%	3.557%
24	11.663	1658	1662	1666	rVB	154691	145058	2.59%	0.341%
25	11.816	1682	1688	1691	rBV	58181	63733	1.14%	0.150%
26	12.145	1738	1744	1745	rBV	78576	75402	1.35%	0.177%
27	12.169	1745	1748	1760	rVB	838887	881816	15.75%	2.070%
28	12.674	1830	1834	1837	rBV	88329	82534	1.47%	0.194%
29	13.145	1911	1914	1921	rVB2	57616	66013	1.18%	0.155%
30	13.398	1945	1957	1960	rBV	3921091	5238327	93.56%	12.296%
31	13.468	1964	1969	1984	rBV	788954	827384	14.78%	1.942%
32	14.545	2149	2152	2159	rBV2	49040	62990	1.13%	0.148%
33	14.621	2161	2165	2168	rBV	508896	567415	10.13%	1.332%
34	14.662	2168	2172	2178	rVB	1293715	1419608	25.36%	3.332%

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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-BF032217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.651	2336	2340	2346	rBV	194549	260409	4.65%	0.611%
36	16.292	2444	2449	2456	rBV	961991	1184935	21.16%	2.782%
37	16.662	2508	2512	2518	rVB2	43219	62627	1.12%	0.147%

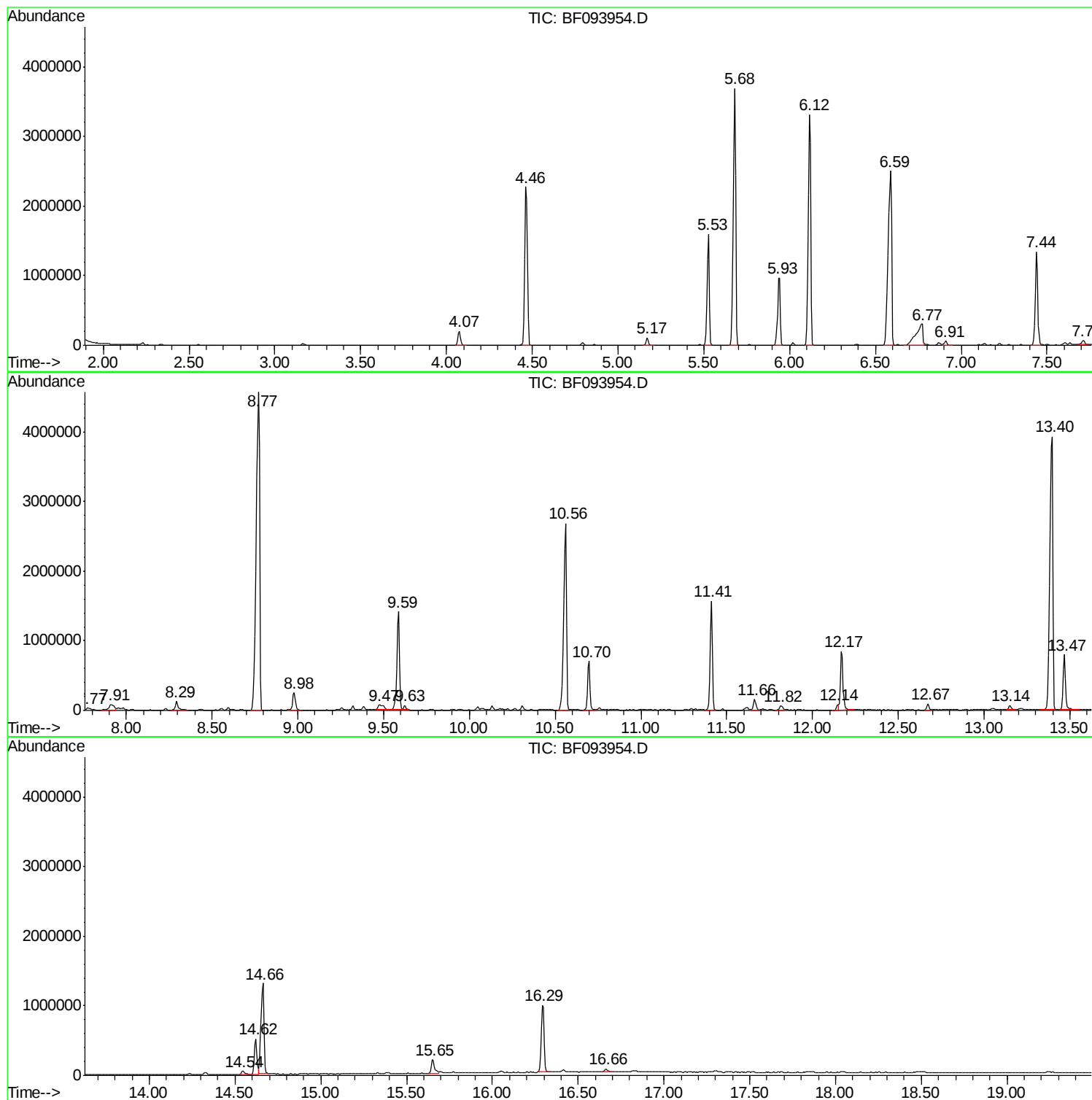
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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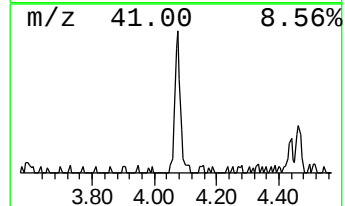
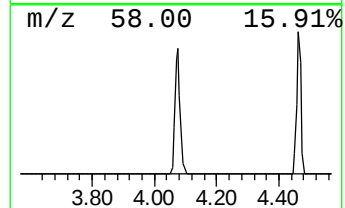
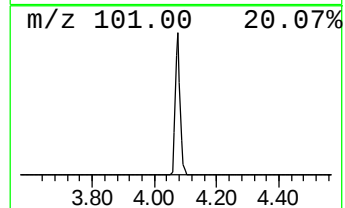
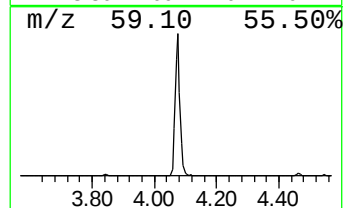
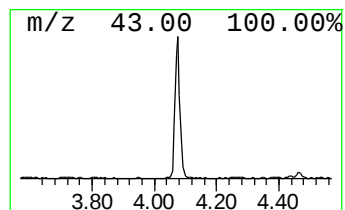
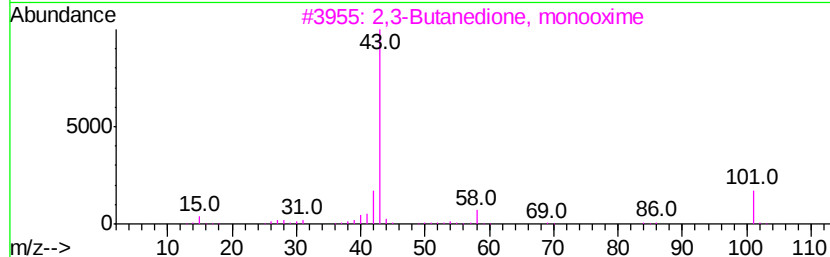
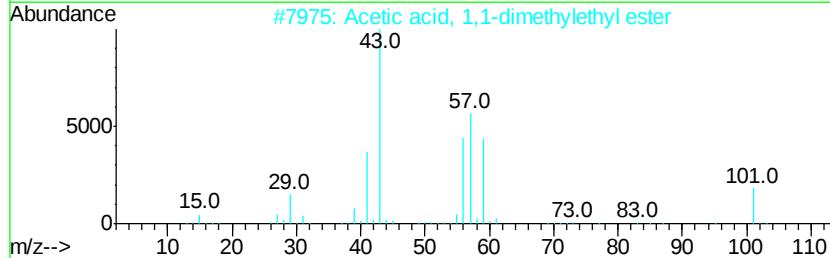
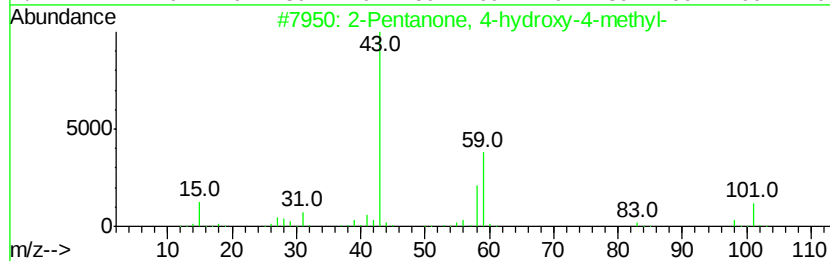
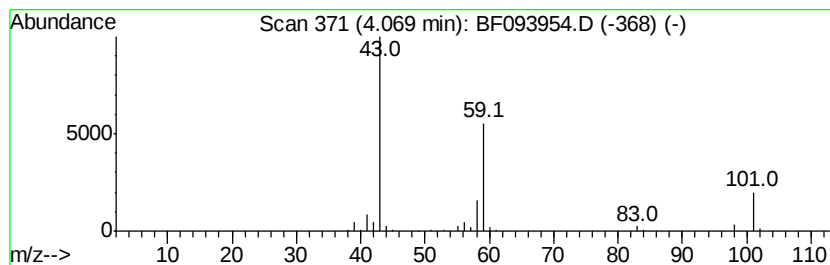
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.07	4.61 ng	227035	1,4-Dichlorobenzene-d4	5.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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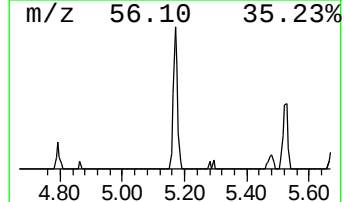
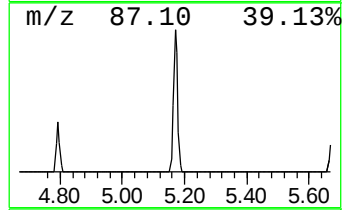
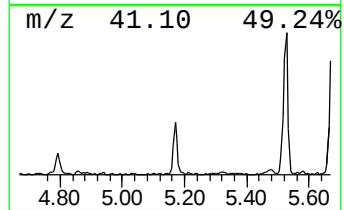
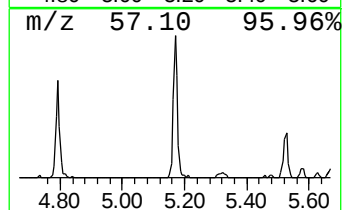
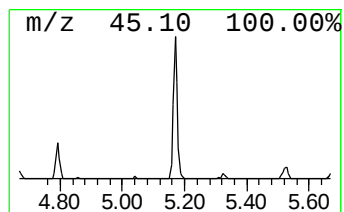
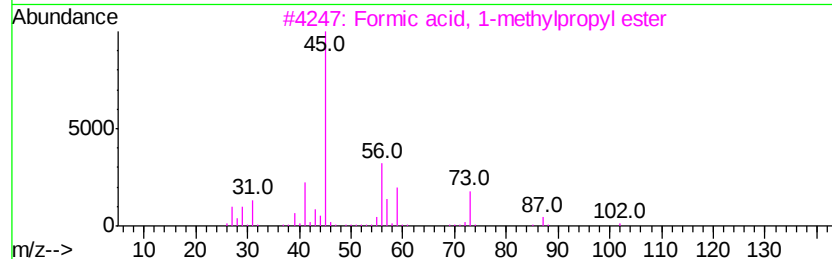
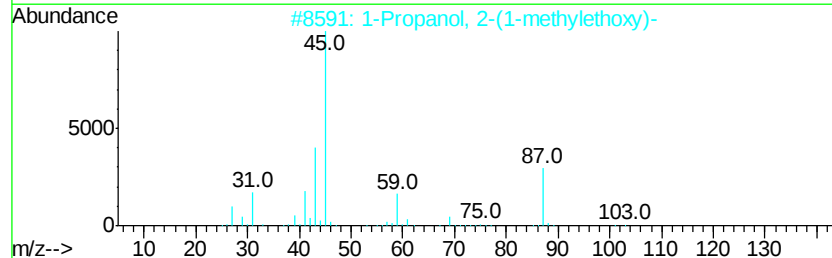
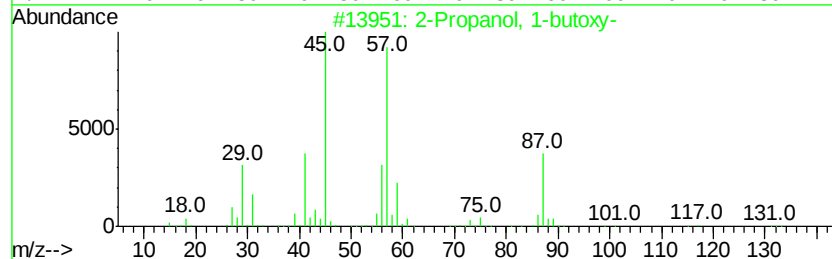
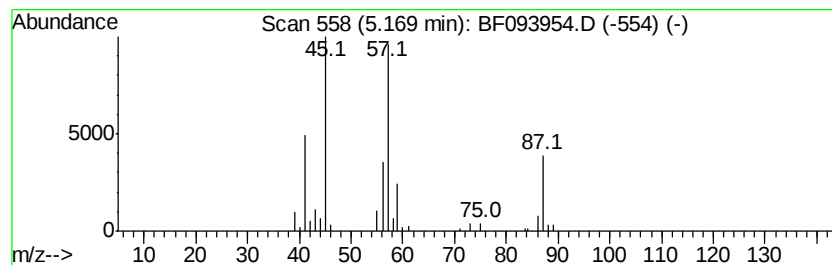
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Propanol, 1-butoxy- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	2.12 ng	104602	1,4-Dichlorobenzene-d4	5.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	74
2			1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	45
3			Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	42
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	40
5			Morpholine	87	C4H9NO	000110-91-8	27



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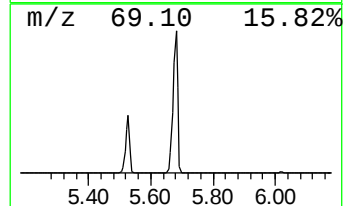
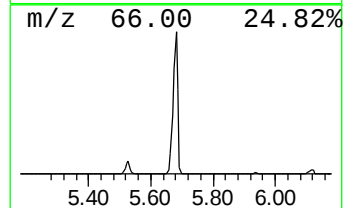
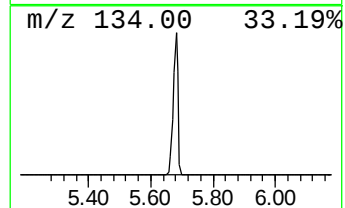
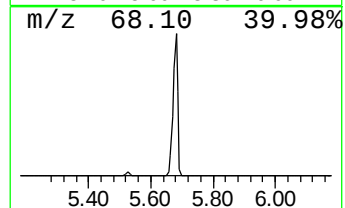
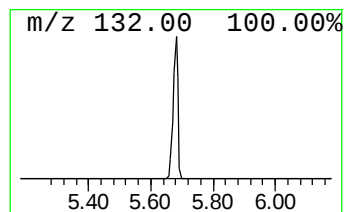
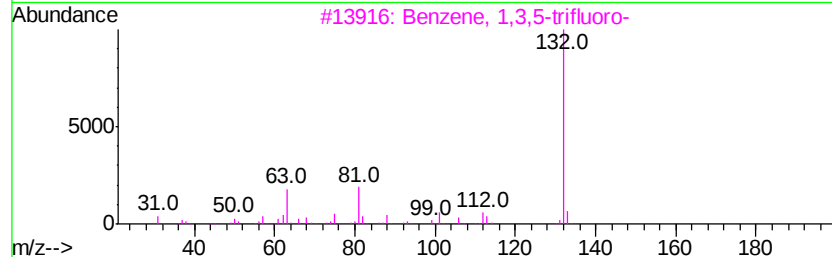
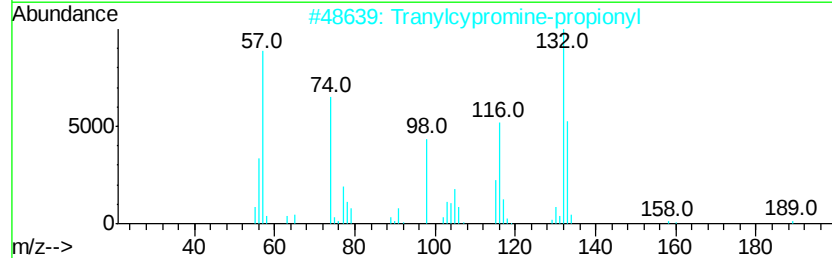
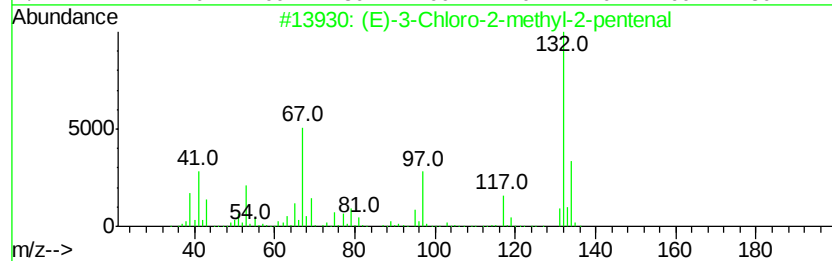
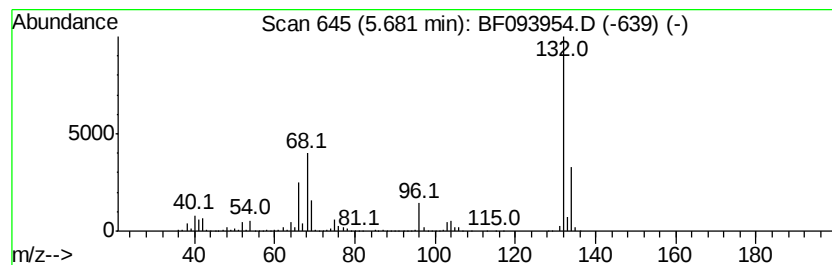
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown5.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.68	80.72 ng	3977900	1,4-Dichlorobenzene-d4	5.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16	
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10	
3	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9	
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9	
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9	



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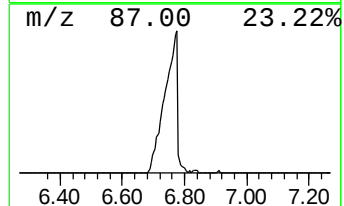
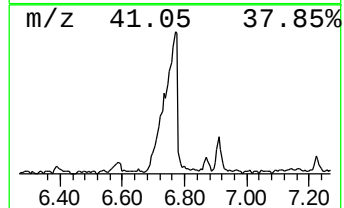
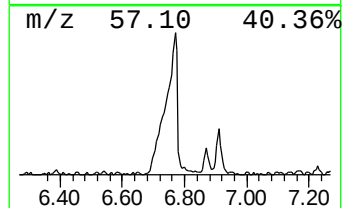
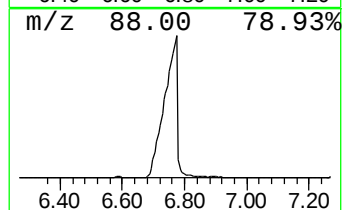
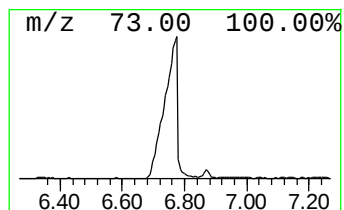
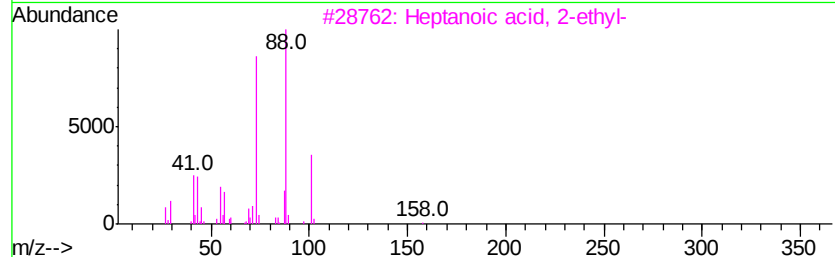
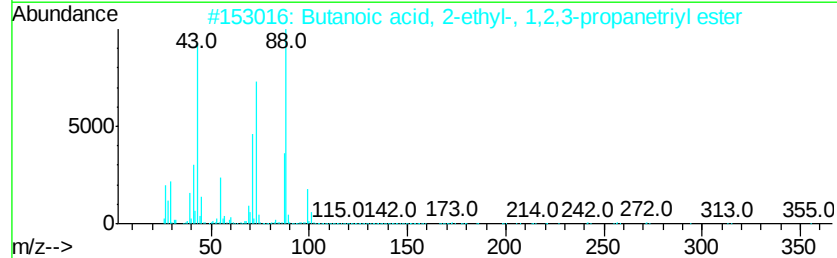
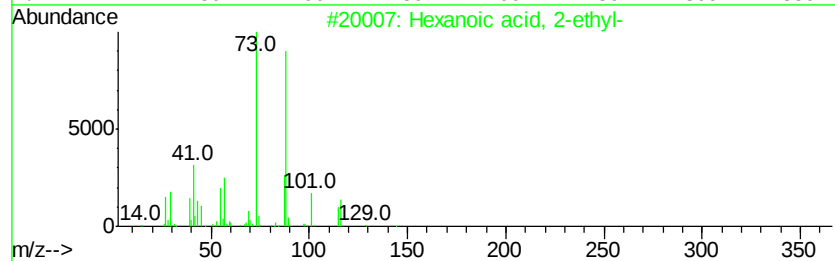
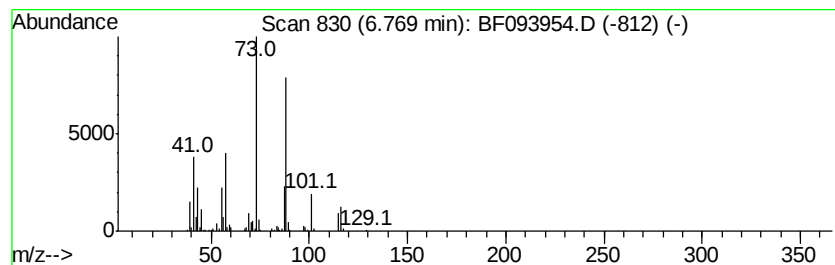
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	12.83 ng	874340	Naphthalene-d8	7.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
3		Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
4		Methyl L-(+)-.beta.-hydroxyvisobu...	118	C5H10O3	080657-57-4	40
5		Octanoic acid, 2-methyl-, methyl...	172	C10H20O2	002177-86-8	38



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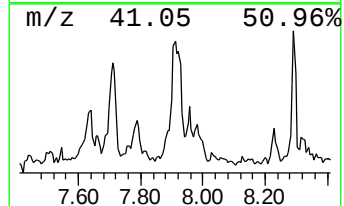
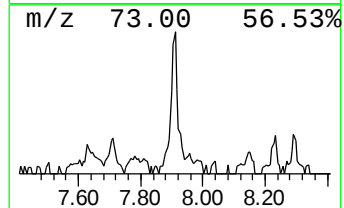
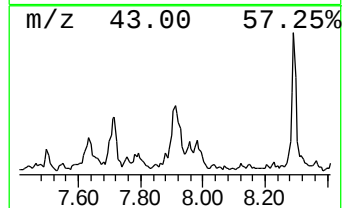
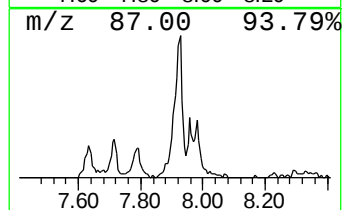
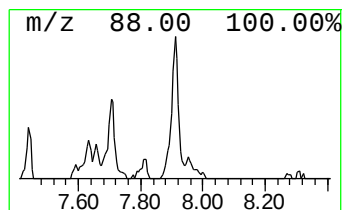
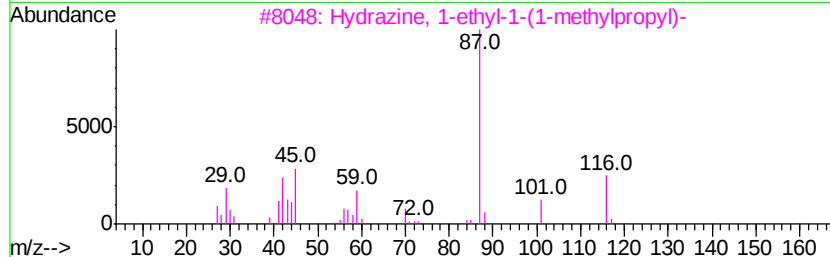
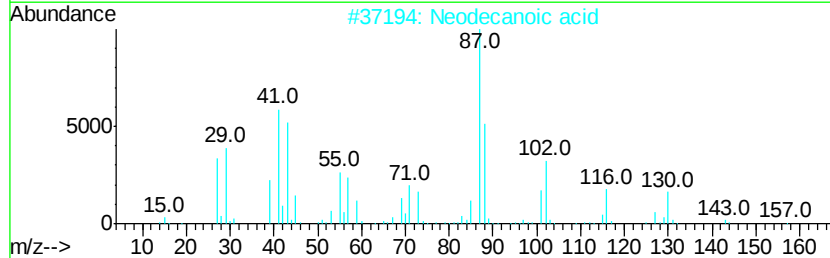
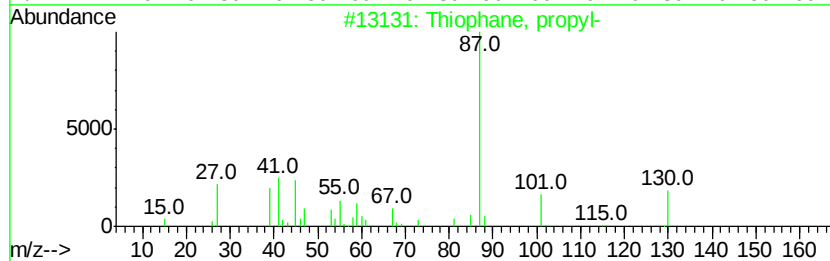
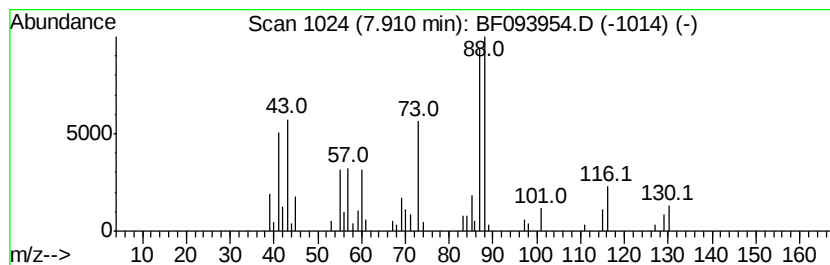
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown7.91 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.91	2.57 ng	174917	Naphthalene-d8	7.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Thiophane, propyl-	130	C7H14S	001551-34-4	43
2		Neodecanoic acid	172	C10H20O2	026896-20-8	40
3		Hvdrazine, 1-ethyl-1-(1-methylpr...	116	C6H16N2	020325-97-7	38
4		Hvdrazine, 1,1-dipropyl-	116	C6H16N2	004986-50-9	35
5		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032717\
Data File : BF093954.D
Acq On : 27 Mar 2017 20:55
Operator : SJ/MA
Sample : I2405-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

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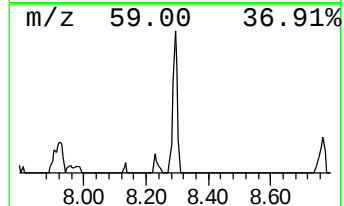
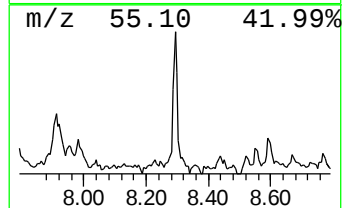
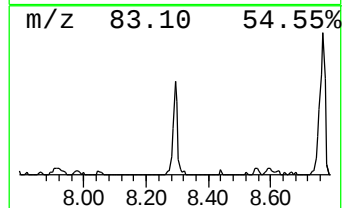
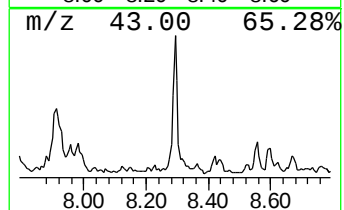
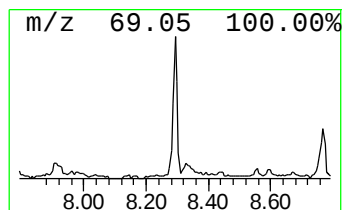
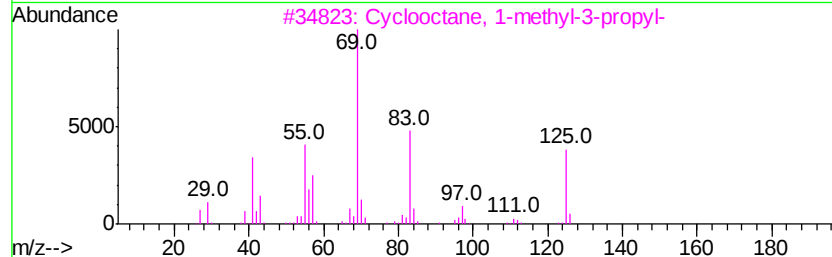
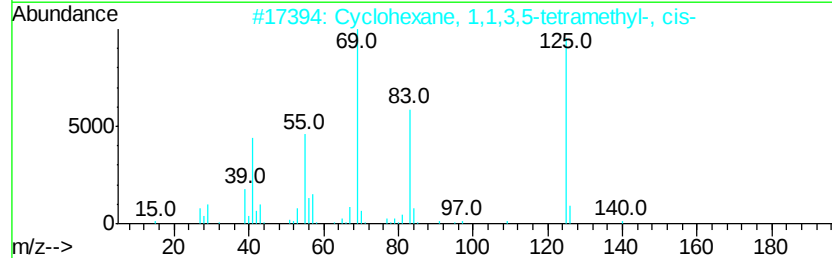
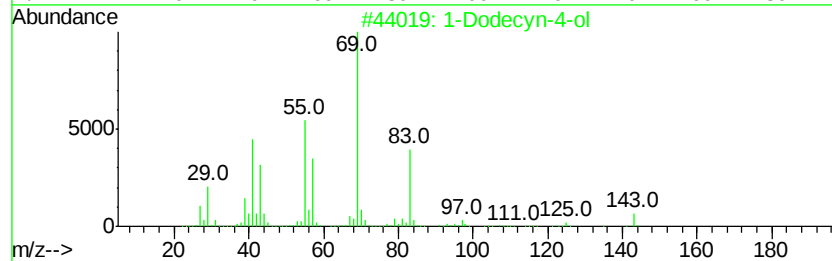
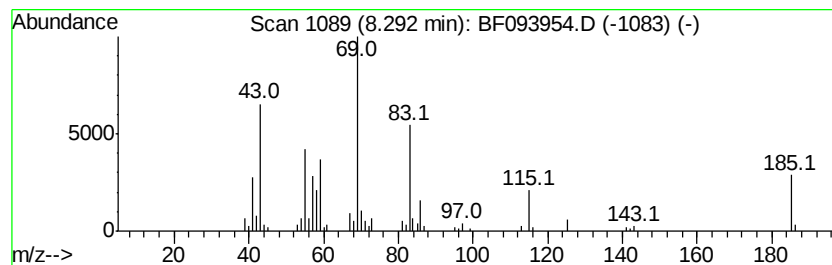
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown8.29 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.29	2.22 ng	151016	Napthalene-d8	7.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Dodecyn-4-ol	182	C12H22O	074646-36-9	37
2		Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	37
3		Cyclooctane, 1-methyl-3-propyl-	168	C12H24	255885-37-1	37
4		Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	37
5		Cyclohexane, 2,4-diethyl-1-methyl-	154	C11H22	061142-70-9	25



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Data File : BF093954.D
Acq On : 27 Mar 2017 20:55
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Sample : I2405-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

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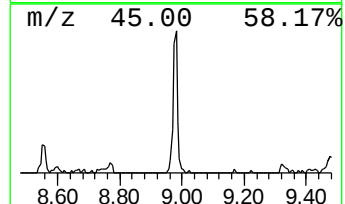
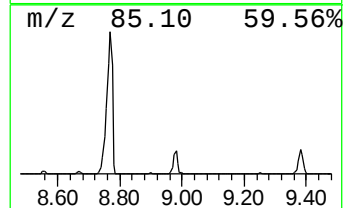
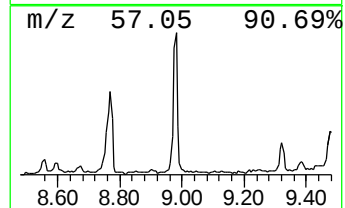
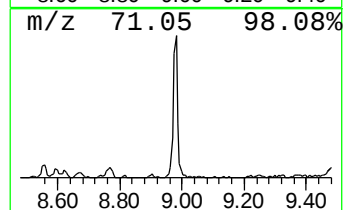
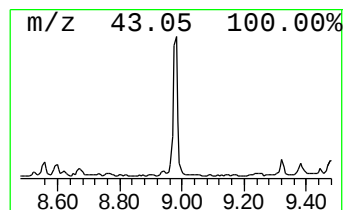
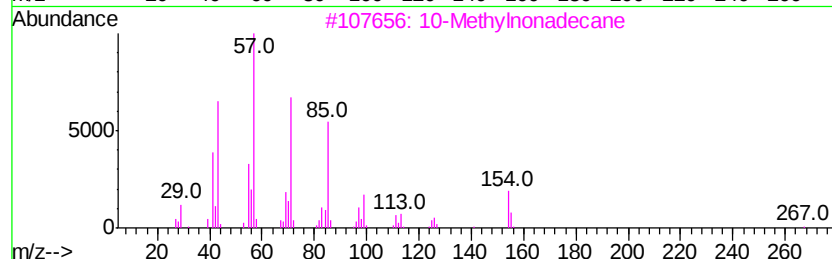
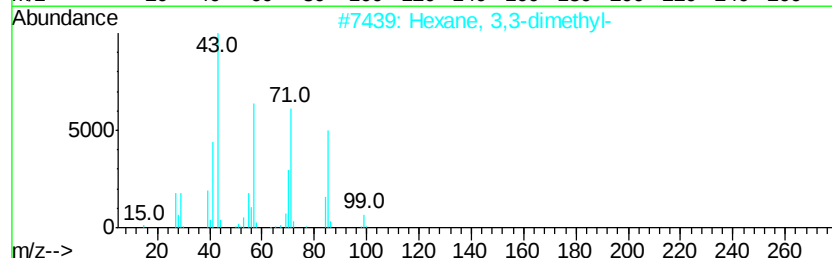
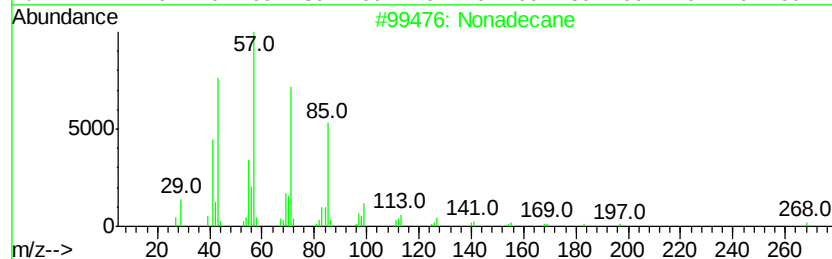
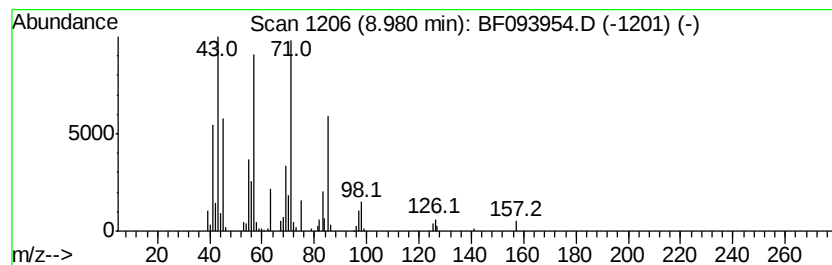
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown8.98 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.98	3.20 ng	244292	Acenaphthene-d10	9.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	47
2		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	43
3		10-Methylnonadecane	282	C20H42	056862-62-5	43
4		Nonane, 5-butyl-	184	C13H28	017312-63-9	38
5		Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032717\
Data File : BF093954.D
Acq On : 27 Mar 2017 20:55
Operator : SJ/MA
Sample : I2405-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

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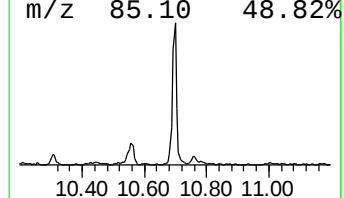
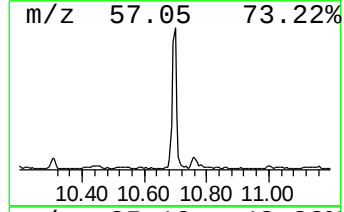
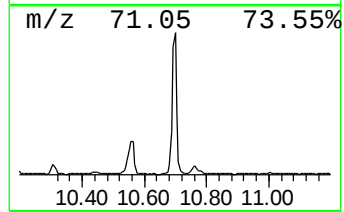
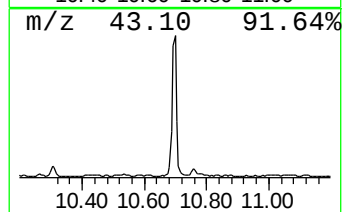
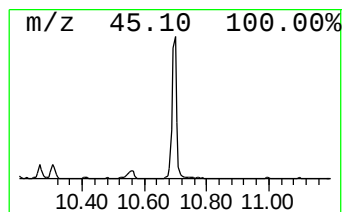
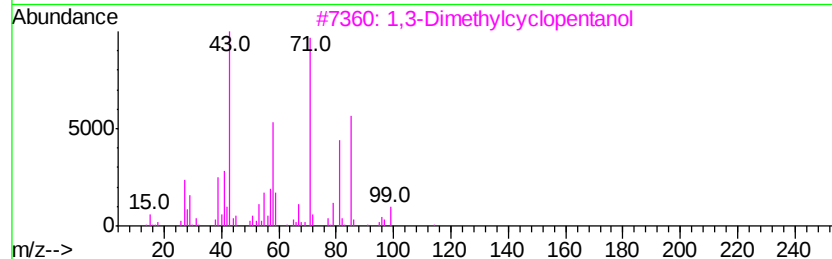
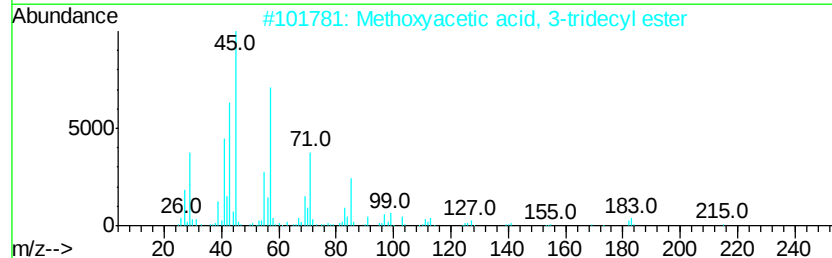
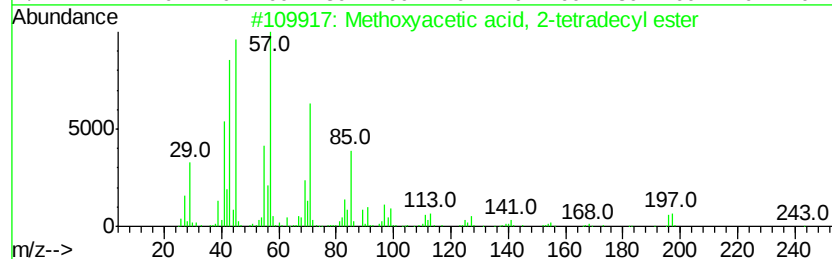
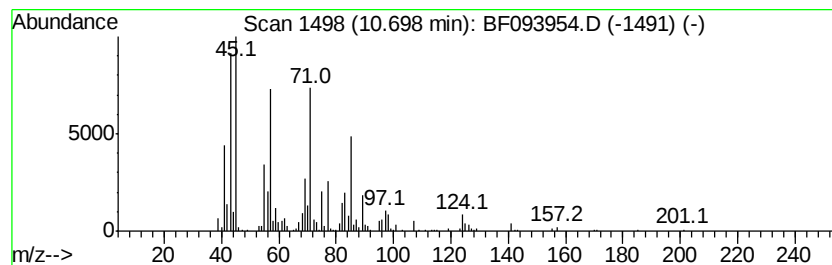
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Methoxyacetic acid, 2-tetra... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	9.31 ng	705567	Phenanthrene-d10	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methoxvacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	53
2		Methoxvacetic acid, 3-tridecyl e...	272	C16H32O3	1000282-04-6	43
3		1,3-Dimethylcyclopentanol	114	C7H14O	019550-46-0	38
4		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	35
5		Octadecane	254	C18H38	000593-45-3	35



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Data File : BF093954.D
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Operator : SJ/MA
Sample : I2405-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

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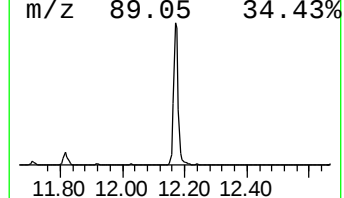
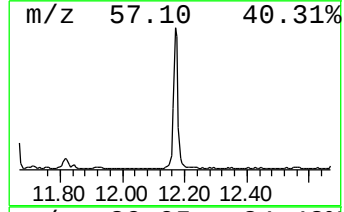
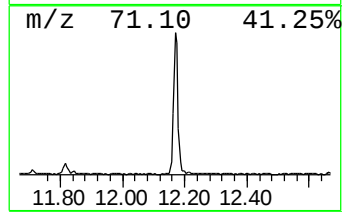
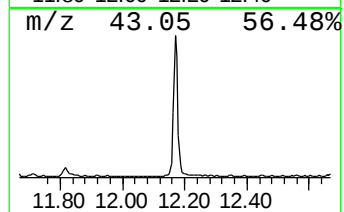
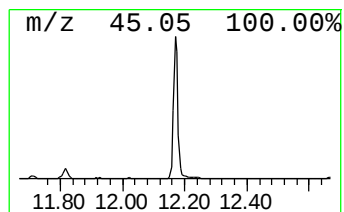
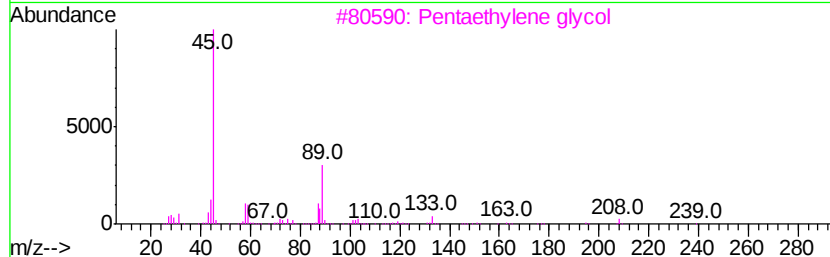
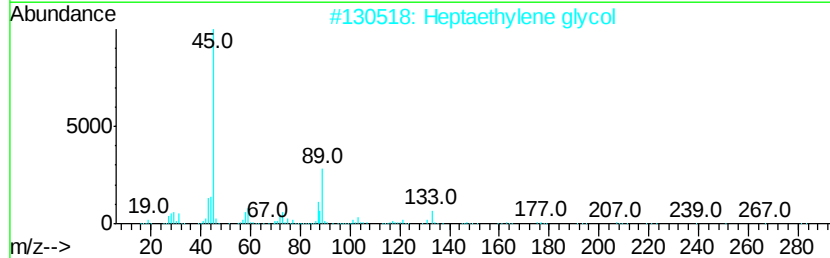
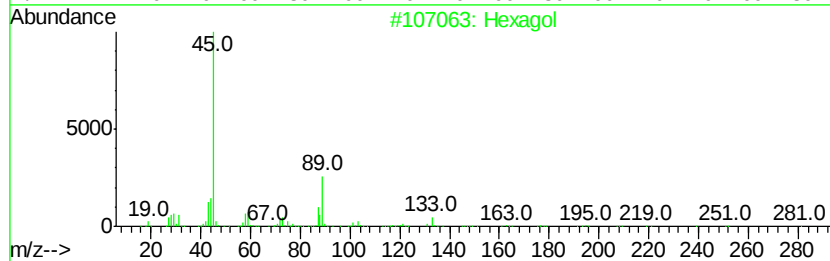
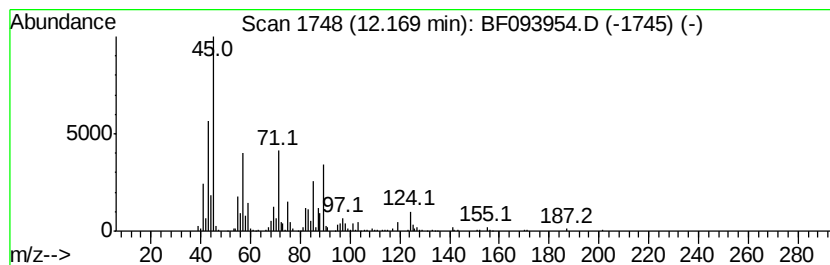
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown12.17 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.17	11.64 ng	881816	Phenanthrene-d10	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexagol	282	C12H26O7	002615-15-8	49
2		Heptaethylene glycol	326	C14H30O8	005617-32-3	49
3		Pentaethylene glycol	238	C10H22O6	004792-15-8	47
4		Ethanol, 2,2'-[oxybis(2,1-ethane...	194	C8H18O5	000112-60-7	47
5		Ethanol, 2-[2-(ethenyloxy)ethoxy]-	132	C6H12O3	000929-37-3	43



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Data File : BF093954.D
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Sample : I2405-02
Misc :
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Instrument :
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ClientSampleId :
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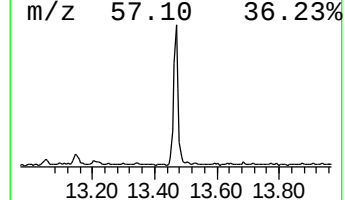
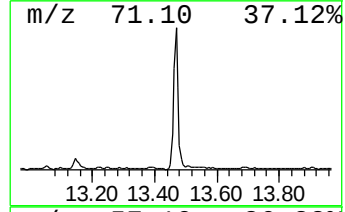
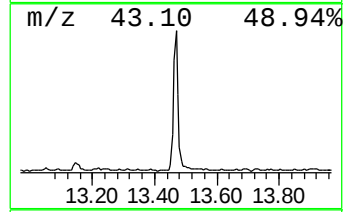
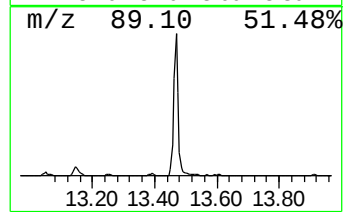
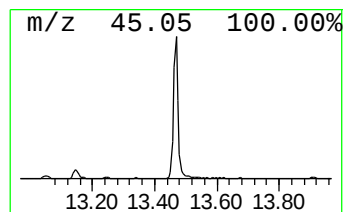
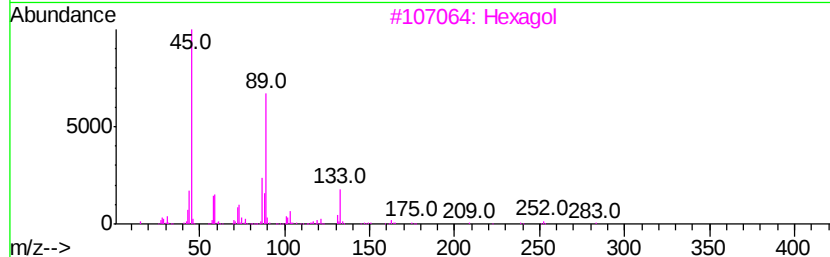
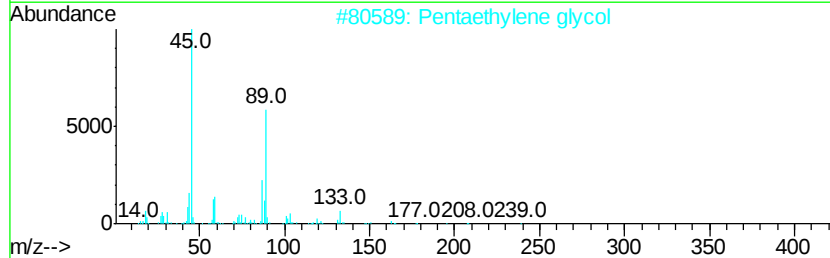
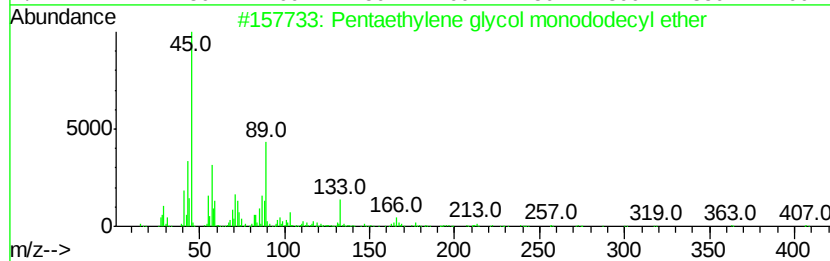
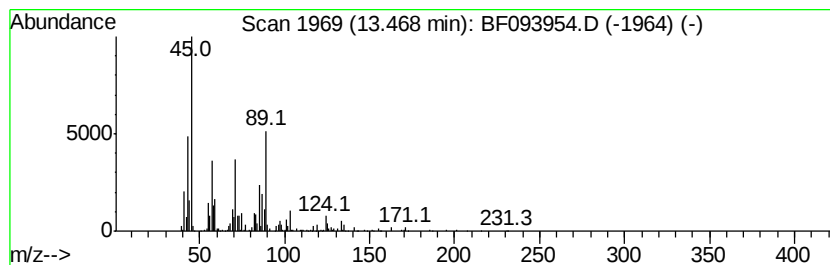
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Pentaethylene glycol monodo... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	11.66 ng	827384	Chrysene-d12	14.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	80
2		Pentaethylene glycol	238	C10H22O6	004792-15-8	64
3		Hexadecyl	282	C12H26O7	002615-15-8	64
4		Octaethylene glycol	370	C16H34O9	1000289-34-2	52
5		Ethanol, 2,2'-[oxybis(2,1-ethane...	194	C8H18O5	000112-60-7	52



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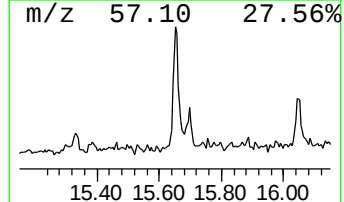
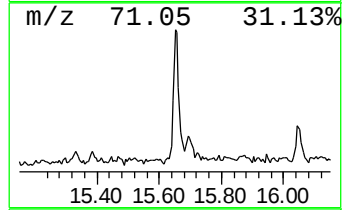
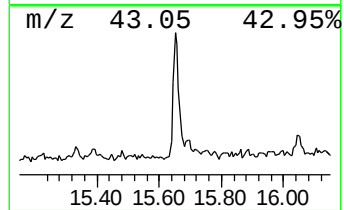
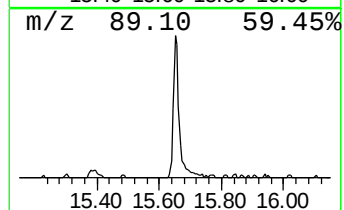
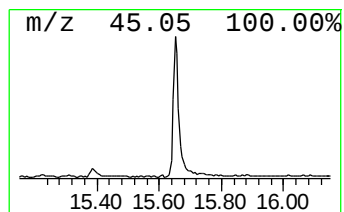
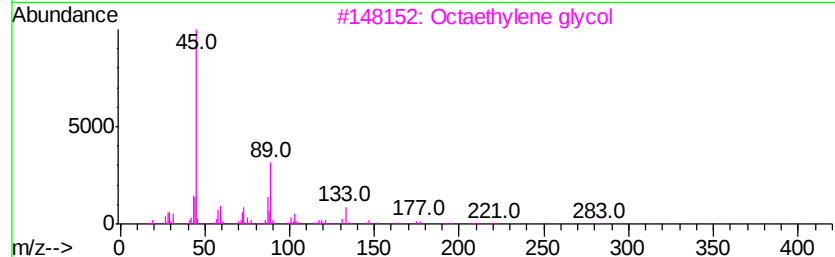
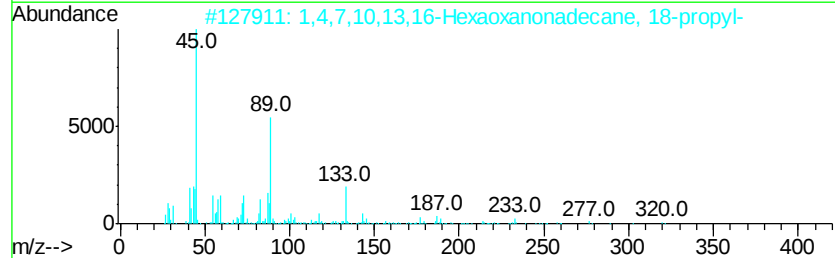
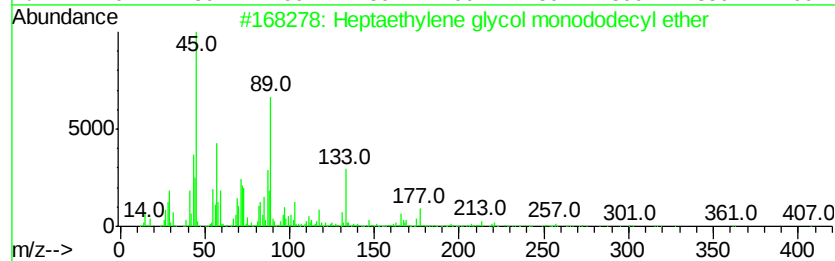
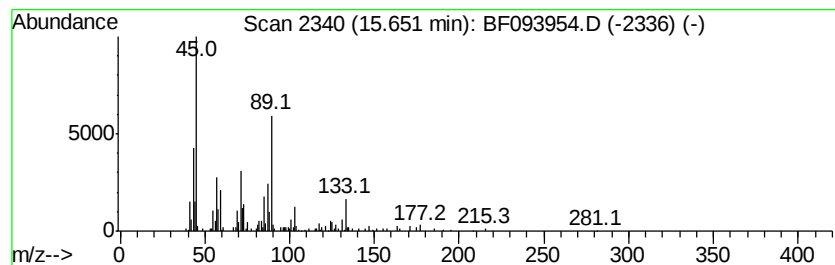
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Heptaethylene glycol monodo... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.65	4.40 ng	260409	Perylene-d12	16.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptaethylene glycol monododecyl...	494	C26H54O8	003055-97-8	72
2			1,4,7,10,13,16-Hexaoxonadecane...	320	C16H32O6	1000163-65-3	72
3			Octaethylene glycol	370	C16H34O9	1000289-34-2	68
4			Hexaethylene glycol monododecyl ...	450	C24H50O7	003055-96-7	64
5			3,6,9,12,15-Pentaoxonadecan-1-ol	294	C14H30O6	001786-94-3	64



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TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.07	4.6 ng		227035	1	5.94	985617	20.0
2-Propanol, 1-but...	5.17	2.1 ng		104602	1	5.94	985617	20.0
unknown5.68	5.68	80.7 ng		3977900	1	5.94	985617	20.0
Hexanoic acid, 2-...	6.77	12.8 ng		874340	2	7.44	1362830	20.0
unknown7.91	7.91	2.6 ng		174917	2	7.44	1362830	20.0
unknown8.29	8.29	2.2 ng		151016	2	7.44	1362830	20.0
unknown8.98	8.98	3.2 ng		244292	3	9.59	1528720	20.0
Methoxyacetic aci...	10.70	9.3 ng		705567	4	11.41	1515260	20.0
unknown12.17	12.17	11.6 ng		881816	4	11.41	1515260	20.0
Pentaethylene gly...	13.47	11.7 ng		827384	5	14.66	1419610	20.0
Heptaethylene gly...	15.65	4.4 ng		260409	6	16.29	1184940	20.0