

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
 Data File : BF095521.D
 Acq On : 28 May 2017 4:14
 Operator : SJ/MA
 Sample : I3244-14
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NM5-COMP-6-18

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-BF050217.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	5.095	533	537	553	rBV	98931	242962	10.32%	1.176%
2	5.701	636	640	686	rBV	810936	2180208	92.59%	10.554%
3	7.283	905	909	925	rBV	828561	1900961	80.73%	9.202%
4	7.401	925	929	947	rVB	1296845	2354581	100.00%	11.398%
5	7.736	982	986	997	rBV	436190	534549	22.70%	2.588%
6	7.972	1021	1026	1046	rBV	1324504	1715821	72.87%	8.306%
7	8.642	1136	1140	1172	rBV	531823	1233209	52.37%	5.970%
8	9.766	1327	1331	1352	rBV	302834	689843	29.30%	3.339%
9	11.530	1626	1631	1657	rBV	1291976	2255776	95.80%	10.920%
10	12.242	1747	1752	1769	rBV	118502	240553	10.22%	1.164%
11	12.595	1807	1812	1832	rBV2	382451	682887	29.00%	3.306%
12	13.424	1948	1953	1958	rVB	31269	35140	1.49%	0.170%
13	13.895	2029	2033	2055	rBV	469637	974422	41.38%	4.717%
14	14.195	2078	2084	2095	rBV2	29186	48455	2.06%	0.235%
15	15.001	2217	2221	2226	rVV	299803	467017	19.83%	2.261%
16	15.042	2226	2228	2238	rVV	104888	189159	8.03%	0.916%
17	15.148	2241	2246	2255	rVB2	14495	32120	1.36%	0.155%
18	15.489	2297	2304	2312	rBV4	21747	54183	2.30%	0.262%
19	15.953	2378	2383	2393	rVB4	50384	99581	4.23%	0.482%
20	16.789	2521	2525	2534	rBV	158794	233770	9.93%	1.132%
21	17.089	2572	2576	2586	rVB	183142	249942	10.62%	1.210%
22	17.312	2610	2614	2622	rBV	1294215	1514281	64.31%	7.330%
23	17.400	2627	2629	2637	rVB4	14133	26322	1.12%	0.127%
24	17.553	2652	2655	2663	rVB2	22704	34455	1.46%	0.167%
25	17.642	2666	2670	2674	rBV2	18329	25295	1.07%	0.122%
26	17.695	2674	2679	2683	rBV4	31389	41460	1.76%	0.201%
27	18.553	2817	2825	2834	rBV5	51986	129849	5.51%	0.629%
28	18.671	2840	2845	2850	rBV2	453543	714002	30.32%	3.456%
29	18.712	2850	2852	2861	rVV3	129373	187024	7.94%	0.905%
30	18.806	2864	2868	2872	rBV3	20563	29965	1.27%	0.145%
31	19.189	2927	2933	2936	rBV2	25318	37637	1.60%	0.182%
32	19.341	2955	2959	2963	rBV4	35309	47074	2.00%	0.228%
33	19.783	3030	3034	3037	rBV2	30009	35541	1.51%	0.172%
34	19.953	3059	3063	3066	rBV	100747	151585	6.44%	0.734%

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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	20.065	3078	3082	3086	rBV	72271	75459	3.20%	0.365%
36	20.241	3109	3112	3117	rBV	61333	69995	2.97%	0.339%
37	20.300	3119	3122	3127	rVB	82086	92197	3.92%	0.446%
38	20.353	3127	3131	3139	rBV	308061	470987	20.00%	2.280%
39	20.794	3202	3206	3211	rVB	54494	68047	2.89%	0.329%
40	21.718	3357	3363	3371	rVB3	105533	198800	8.44%	0.962%
41	21.865	3383	3388	3394	rVB8	36173	74799	3.18%	0.362%
42	22.106	3425	3429	3435	rBV2	27660	63052	2.68%	0.305%
43	22.971	3568	3576	3582	rVB10	25394	66212	2.81%	0.321%
44	23.324	3630	3636	3644	rVB6	36780	88344	3.75%	0.428%

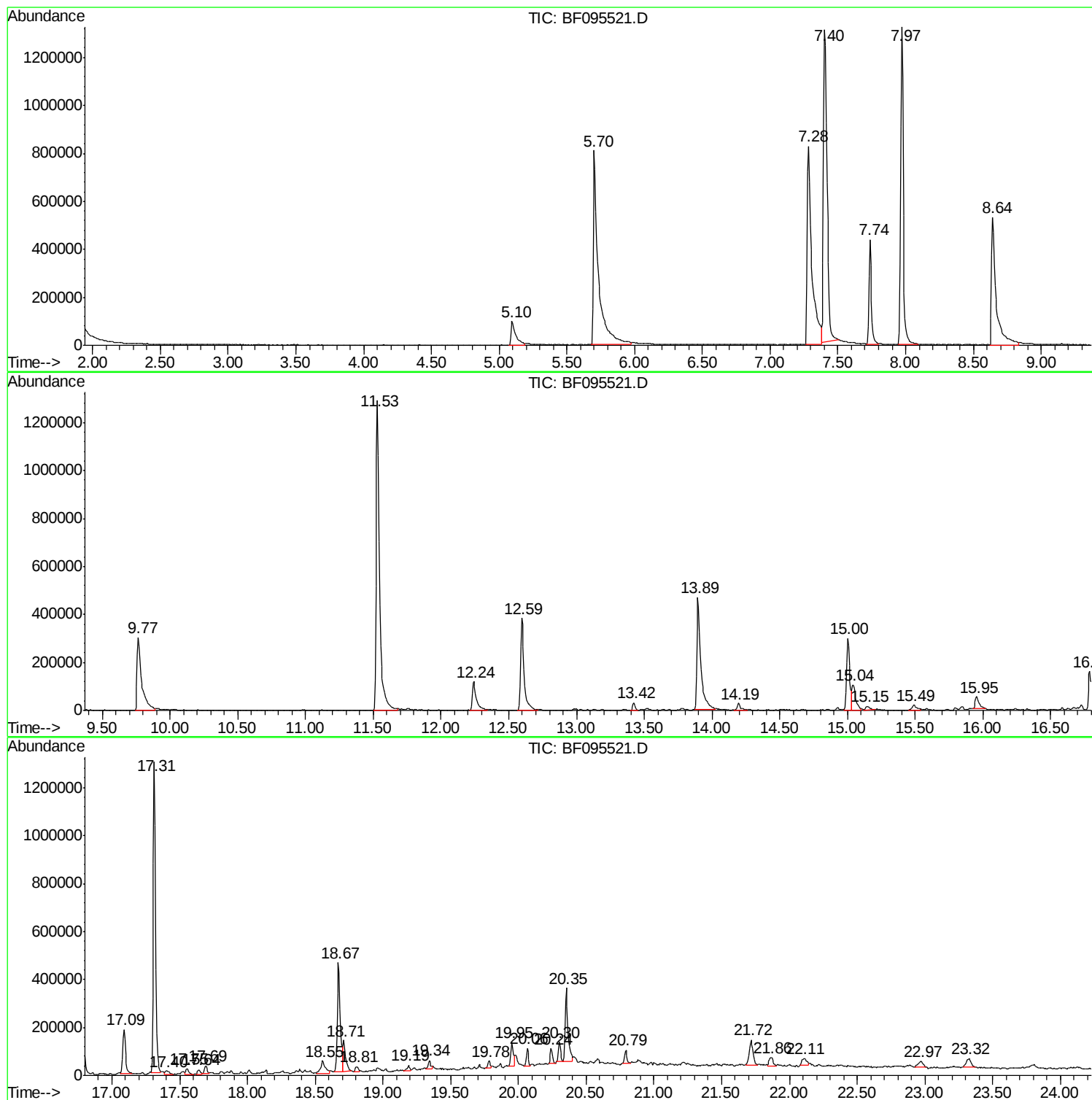
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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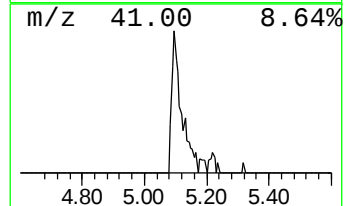
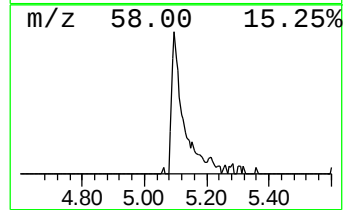
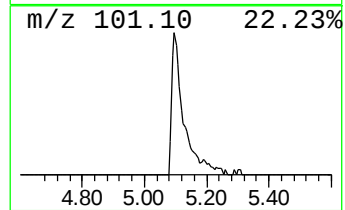
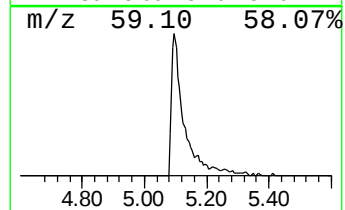
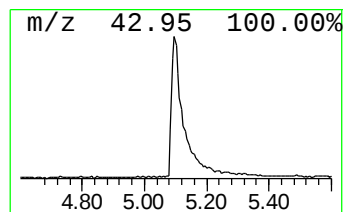
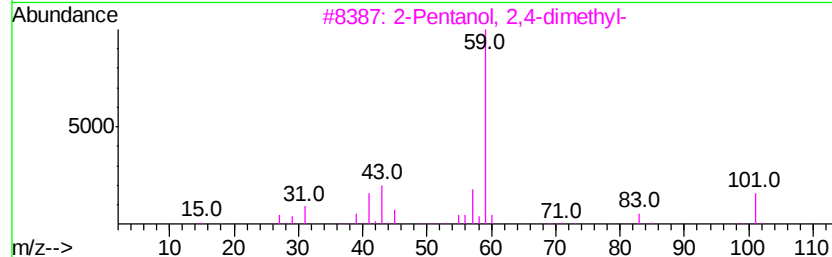
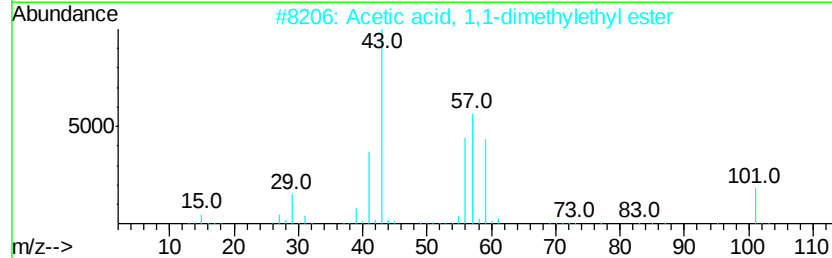
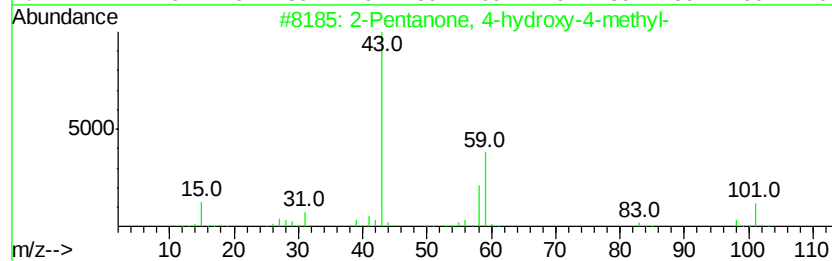
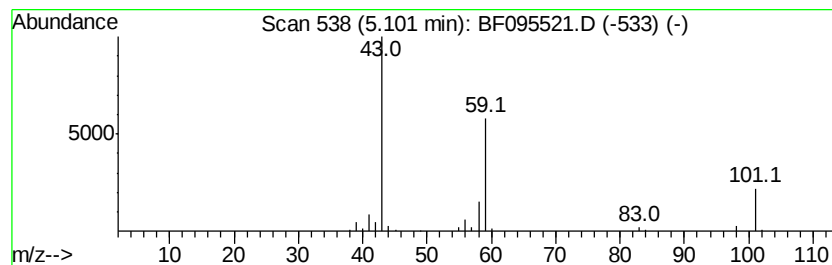
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	9.09 ng	242962	1,4-Dichlorobenzene-d4	7.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	25
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Acetone	58	C3H6O	000067-64-1	9



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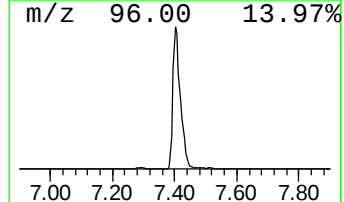
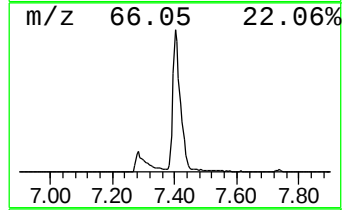
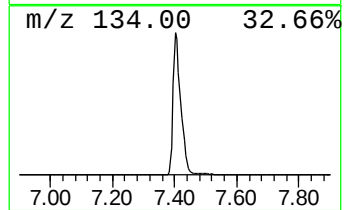
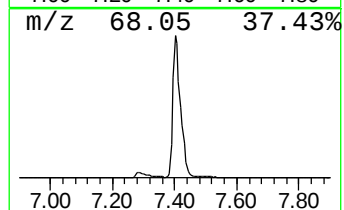
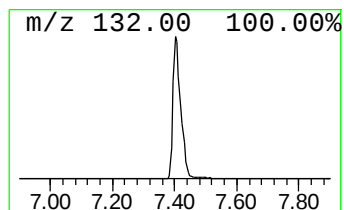
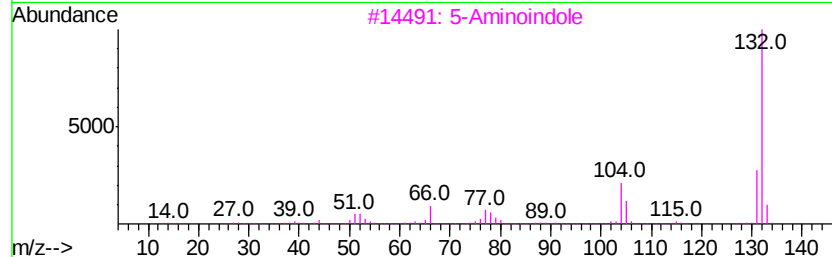
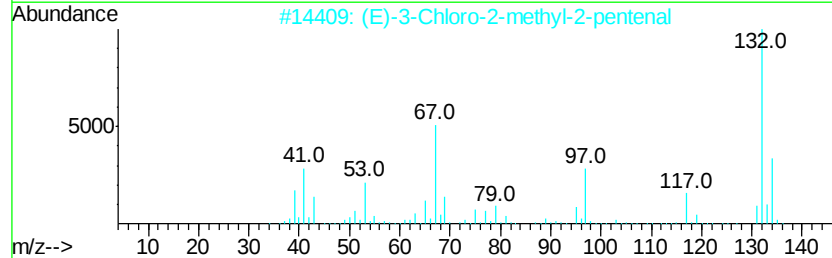
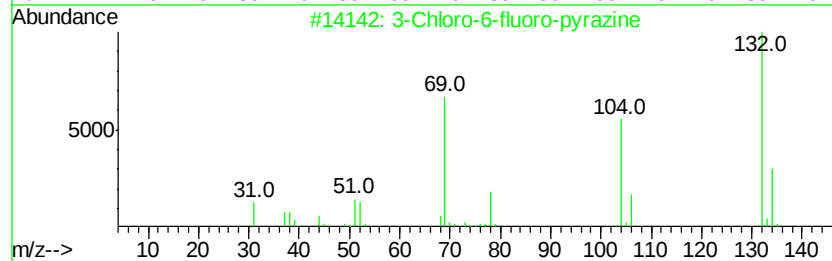
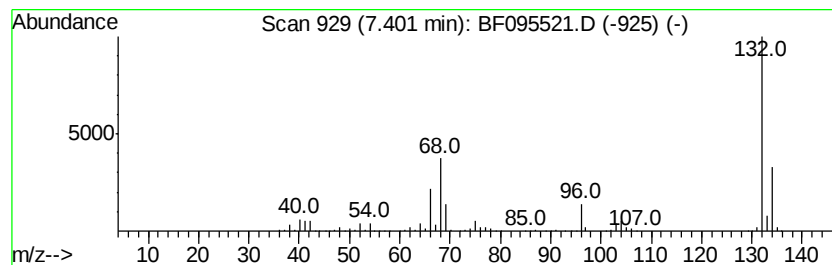
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Peak Number 2 unknown7.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.40	88.10 ng	2354580	1,4-Dichlorobenzene-d4	7.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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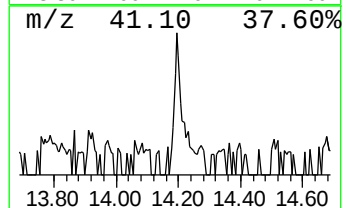
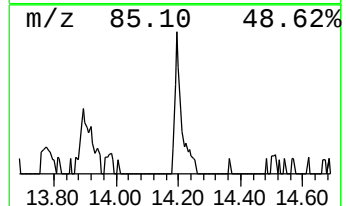
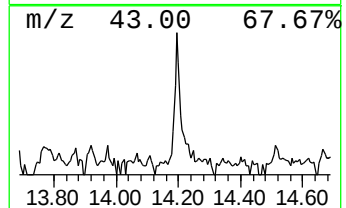
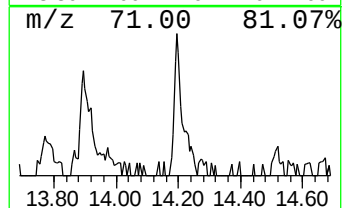
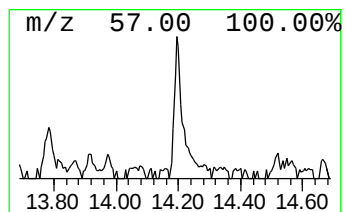
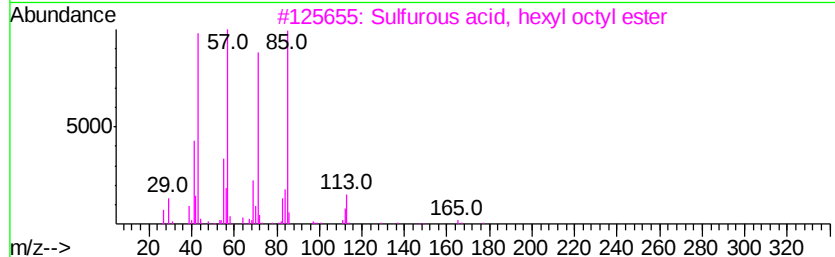
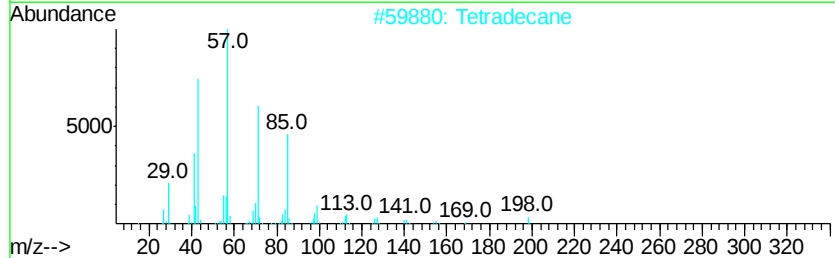
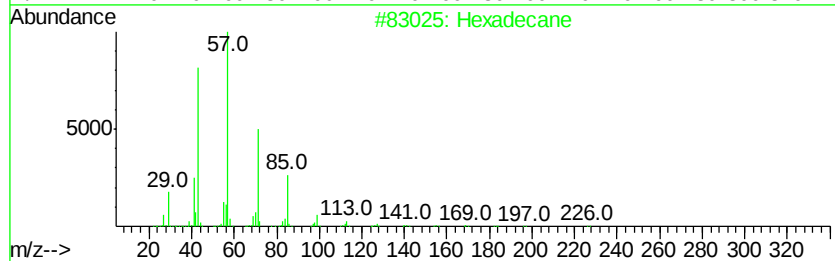
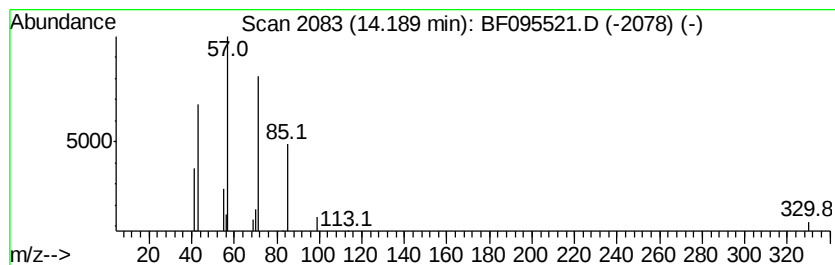
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	2.08 ng	48455	Phenanthrene-d10	15.00
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	78
2	Tetradecane	198 C14H30	000629-59-4	72
3	Sulfurous acid, hexyl octyl ester	278 C14H30O3S	1000309-13-0	64
4	3-Ethyl-3-methylheptane	142 C10H22	017302-01-1	59
5	Sulfurous acid, hexyl heptyl ester	264 C13H28O3S	1000309-12-9	53



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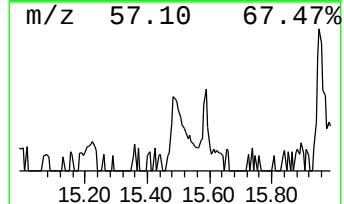
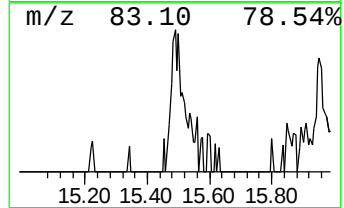
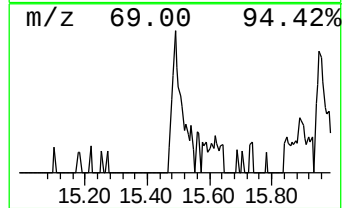
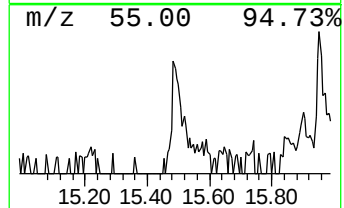
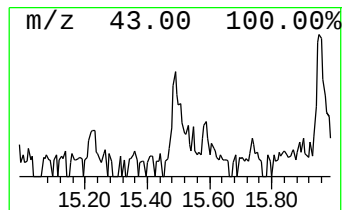
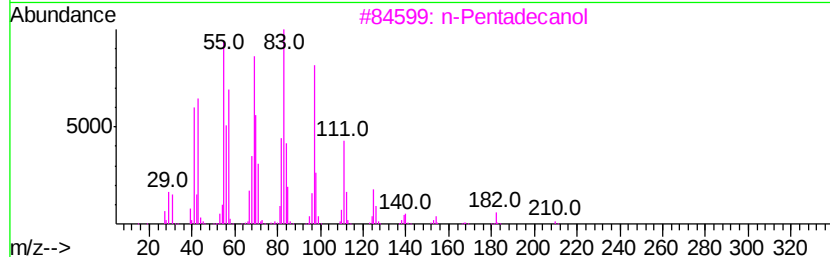
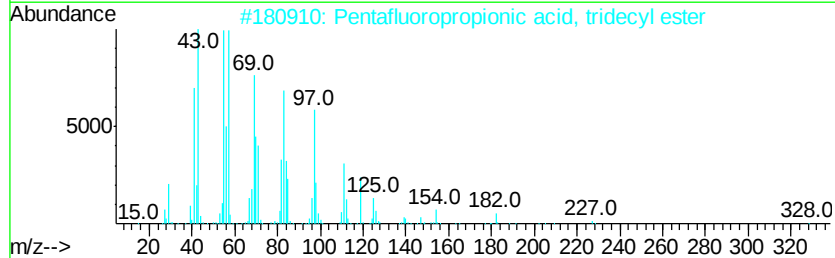
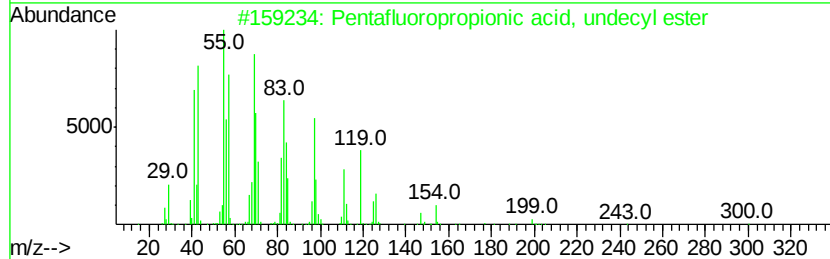
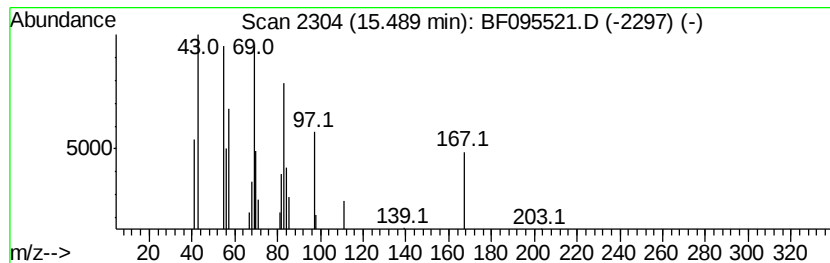
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.49	2.32 ng	54183	Phenanthrene-d10	15.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentafluoropropionic acid, undec...	318	C14H23F5O2	959014-11-0	90
2		Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	86
3		n-Pentadecanol	228	C15H32O	000629-76-5	83
4		1-Tetradecanol	214	C14H30O	000112-72-1	83
5		n-Tridecan-1-ol	200	C13H28O	000112-70-9	83



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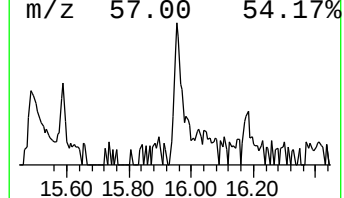
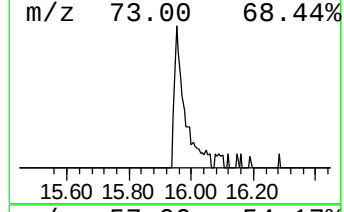
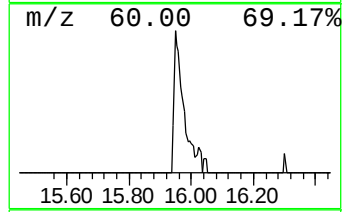
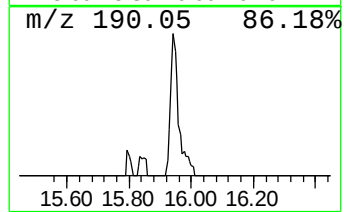
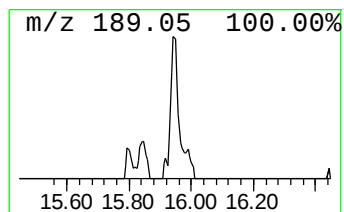
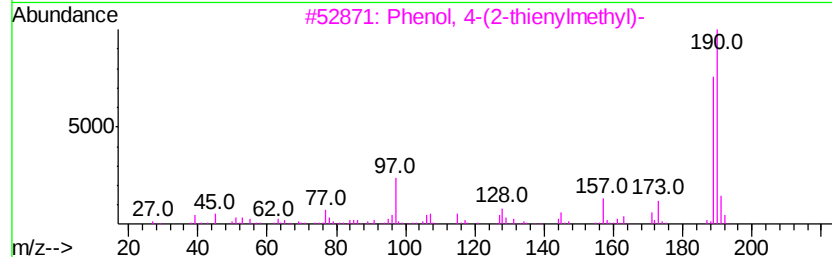
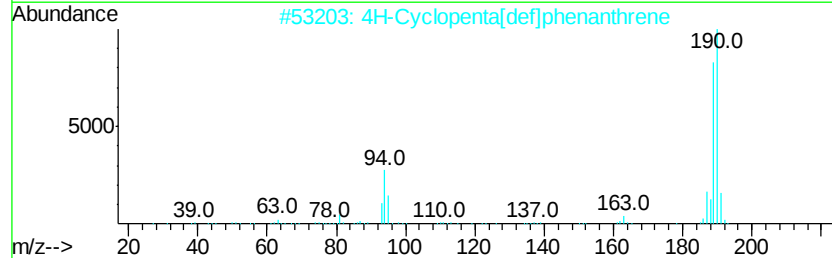
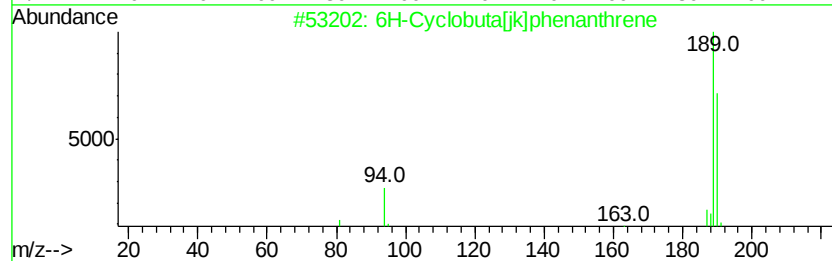
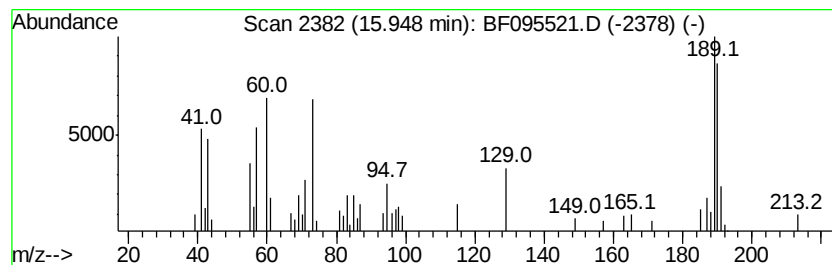
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ClientSampleId :
NM5-COMP-6-18

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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 6 6H-Cyclobuta[jk]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD			R.T.
15.95	4.26 ng	99581	Phenanthrene-d10			15.00
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6H-Cyclobuta[ik]phenanthrene	190	C15H10		083469-43-6	58
2	4H-Cyclopenta[def]phenanthrene	190	C15H10		000203-64-5	47
3	Phenol, 4-(2-thienylmethyl)-	190	C11H10OS		091680-55-6	43
4	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BCl03S		036155-87-0	38
5	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2		000090-60-8	32



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
Data File : BF095521.D
Acq On : 28 May 2017 4:14
Operator : SJ/MA
Sample : I3244-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NM5-COMP-6-18

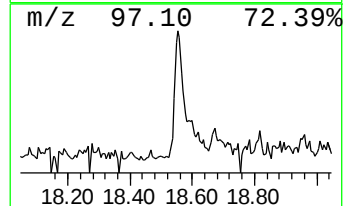
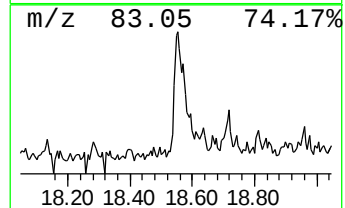
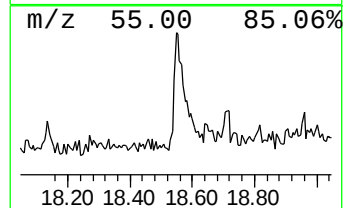
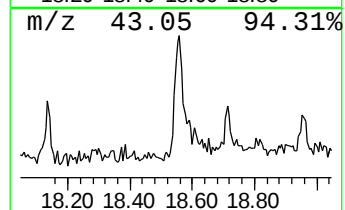
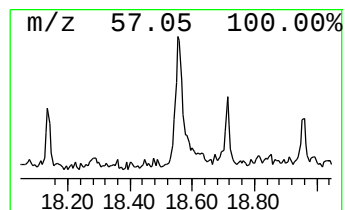
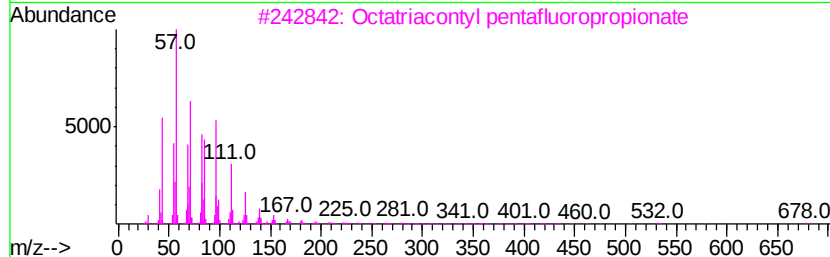
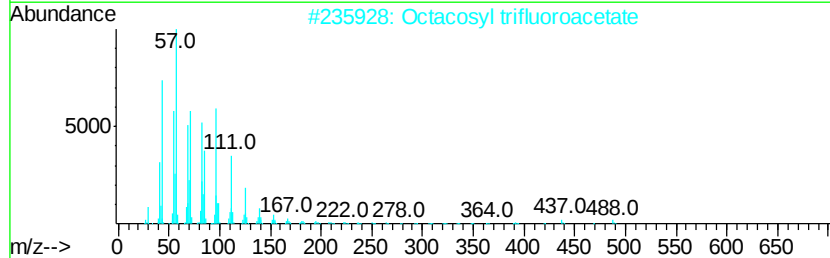
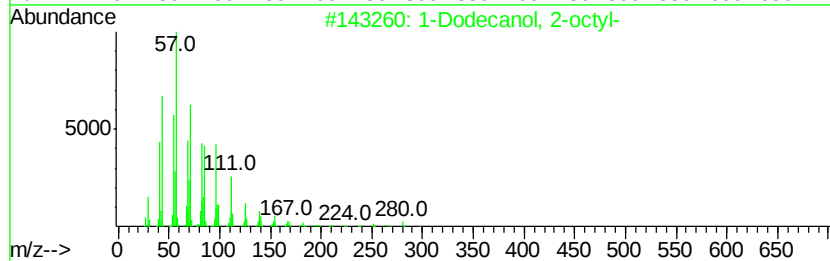
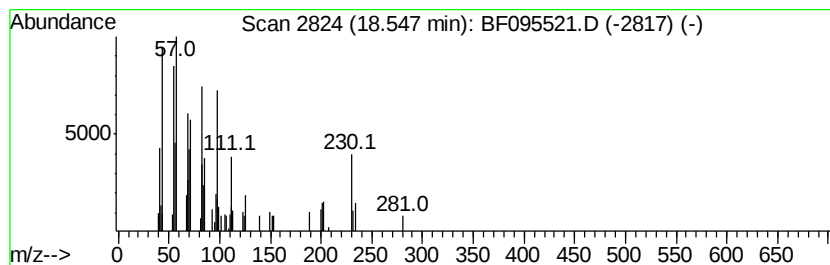
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Dodecanol, 2-octyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.55	3.64 ng	129849	Chrysene-d12	18.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	83
2		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	76
3		Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	68
4		Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	64
5		Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
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ClientSampleId :
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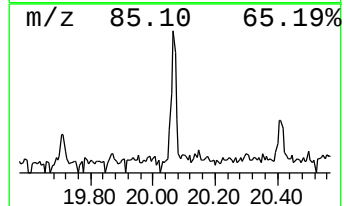
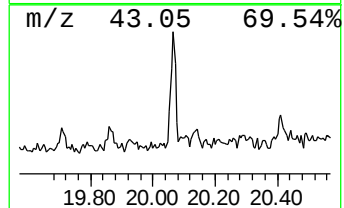
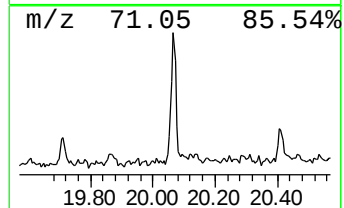
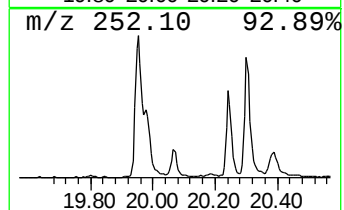
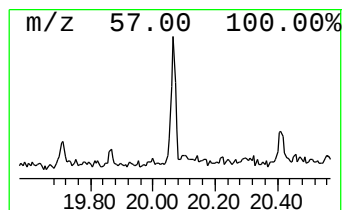
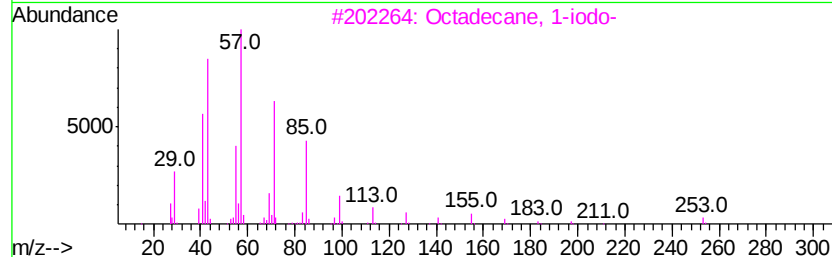
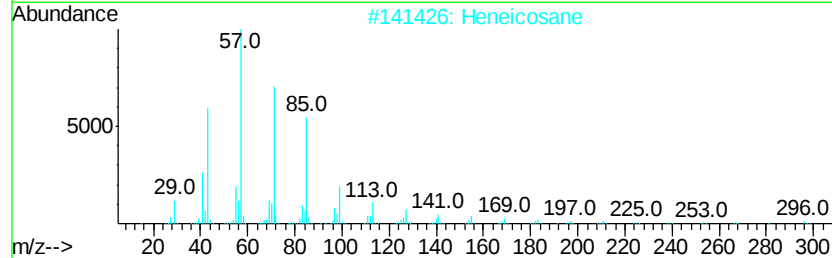
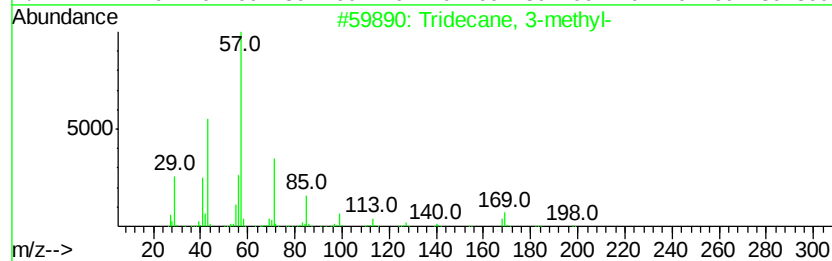
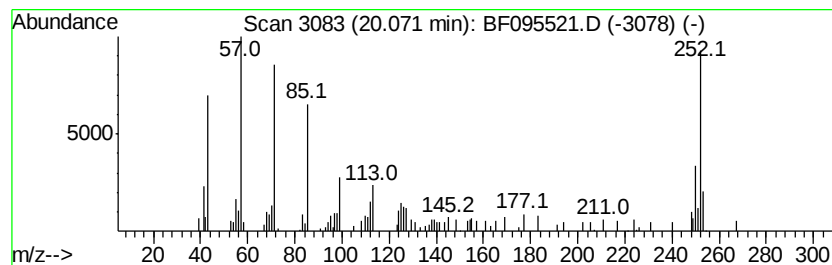
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown20.07 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.07	3.20 ng	75459	Perylene-d12	20.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane, 3-methyl-	198	C14H30	006418-41-3	45
2		Heneicosane	296	C21H44	000629-94-7	45
3		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	43
4		Hexadecane	226	C16H34	000544-76-3	43
5		Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052717\
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Operator : SJ/MA
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Misc :
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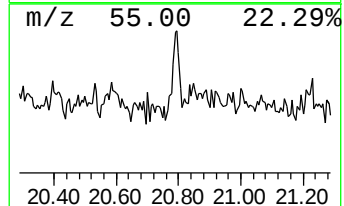
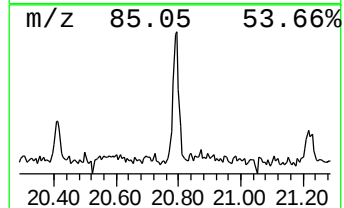
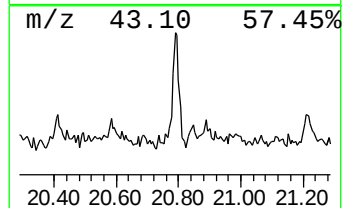
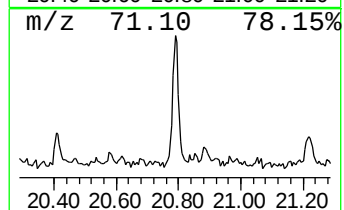
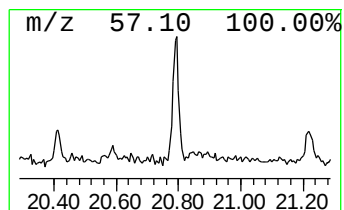
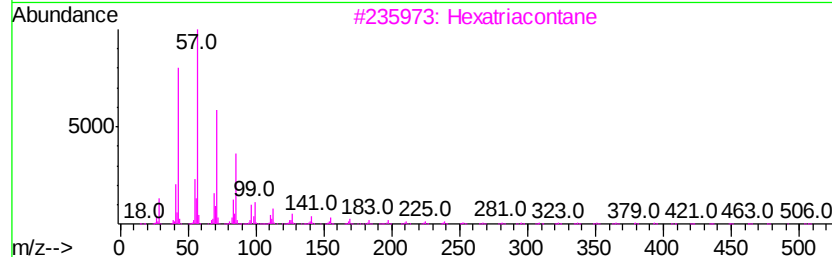
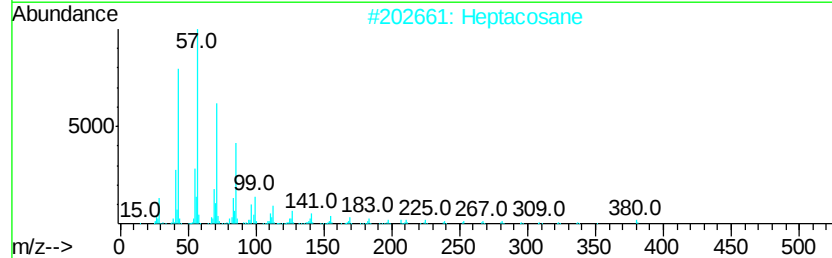
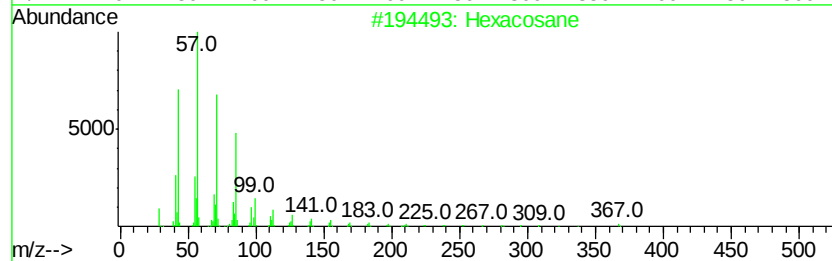
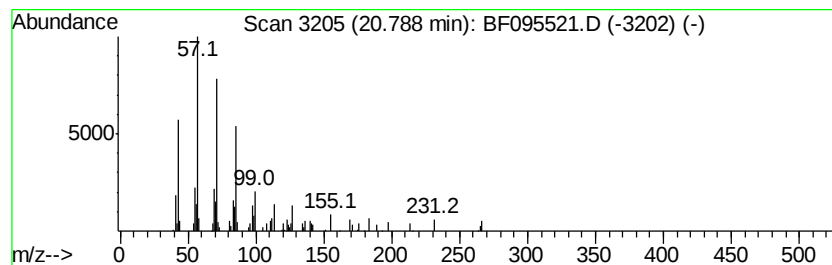
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.79	2.89 ng	68047	Perylene-d12	20.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	90
2			Heptacosane	380	C27H56	000593-49-7	90
3			Hexatriacontane	507	C36H74	000630-06-8	87
4			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
5			Heptadecane	240	C17H36	000629-78-7	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
Data File : BF095521.D
Acq On : 28 May 2017 4:14
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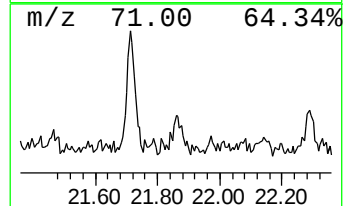
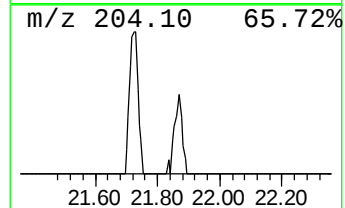
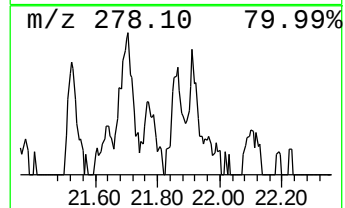
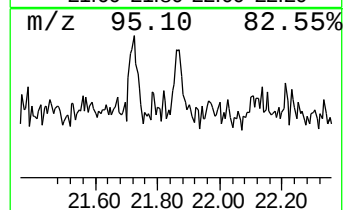
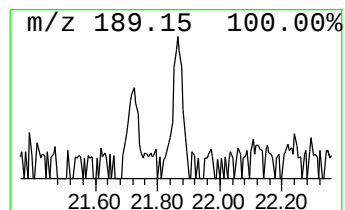
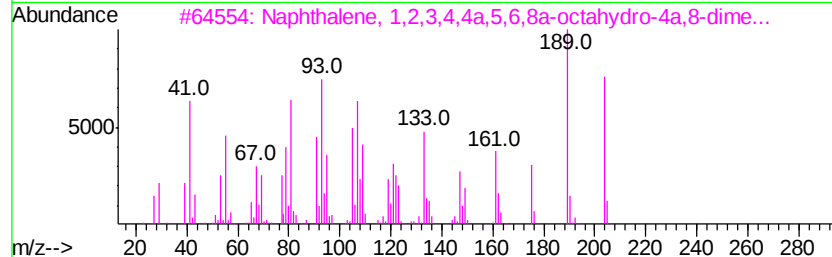
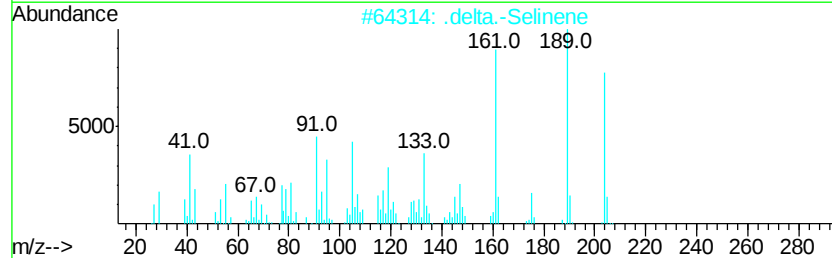
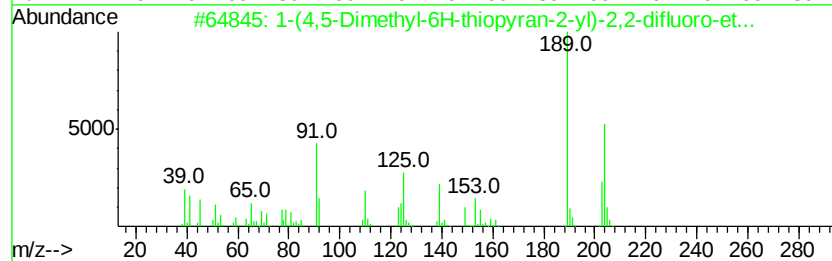
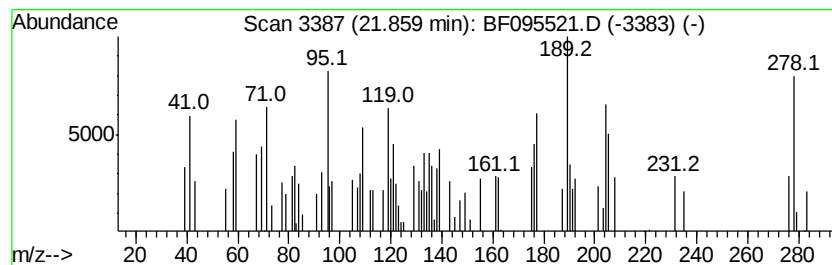
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown21.86 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.86	3.18 ng	74799	Perylene-d12	20.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-(4,5-Dimethyl-6H-thiopyran-2-v...	204	C9H10F2OS	1000318-25-0	20
2		.delta.-Selinene	204	C15H24	028624-23-9	18
3		Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	18
4		1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	18
5		2,10,10-Trimethyltricyclo[7.1.1...	204	C14H200	1000210-81-9	18



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
Data File : BF095521.D
Acq On : 28 May 2017 4:14
Operator : SJ/MA
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Instrument :
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ClientSampleId :
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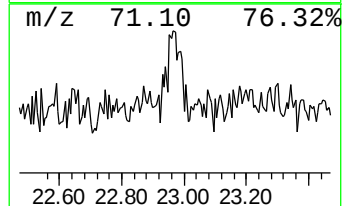
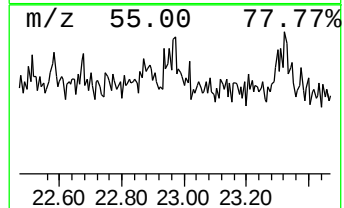
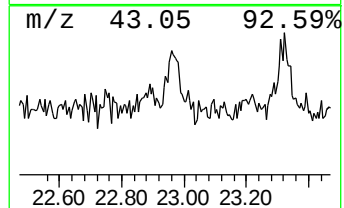
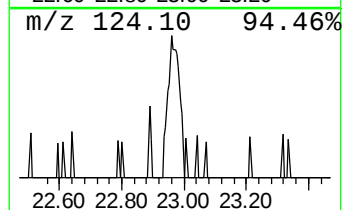
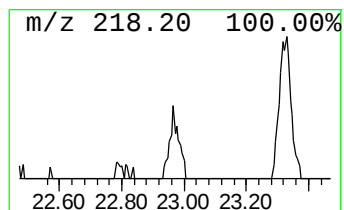
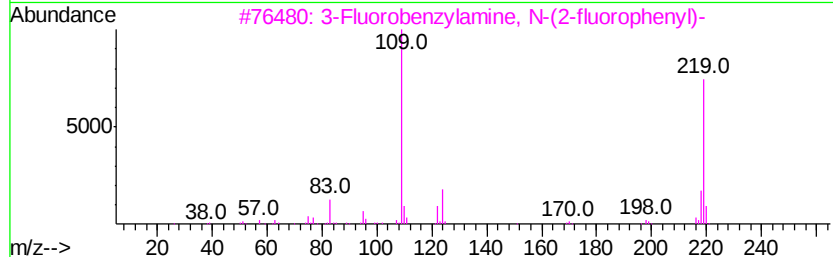
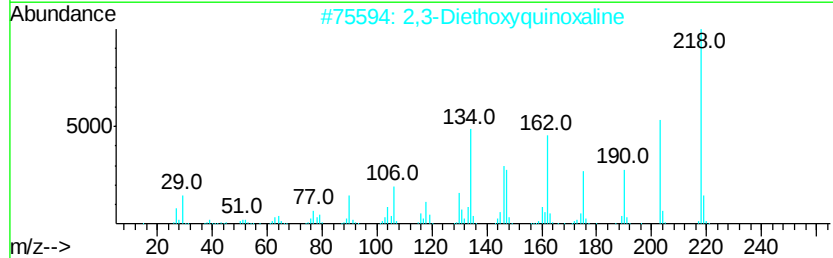
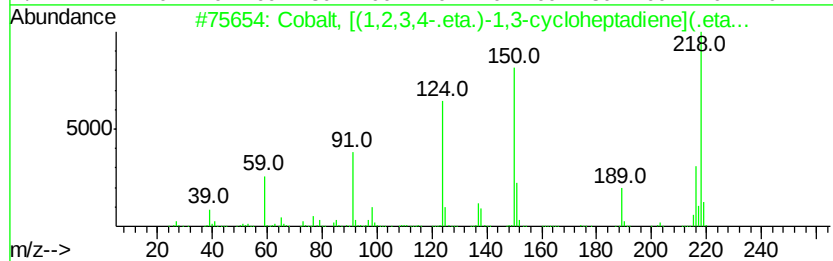
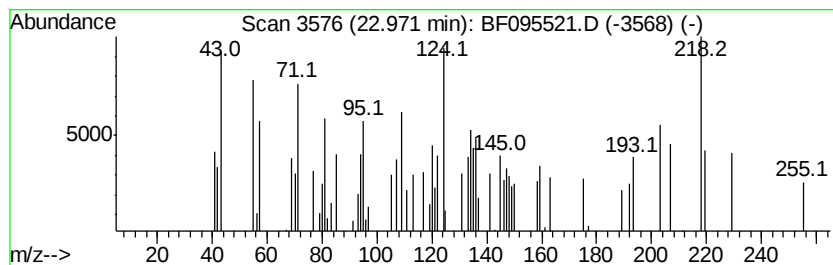
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown22.97 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.97	2.81 ng	66212	Perylene-d12	20.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cobalt, [(1,2,3,4-.eta.)-1,3-cvc...	218	C12H15Co	070210-70-7	12
2		2,3-Diethoxyquinoxaline	218	C12H14N2O2	057050-66-5	11
3		3-Fluorobenzvlamine, N-(2-fluoro...	219	C13H11F2N	1000310-45-4	10
4		3,5-Dimethylphenyl 2,2,2-trifluo...	218	C10H9F3O2	1000373-26-3	10
5		Cyclopenta[c]pyran-7-carboxaldeh...	218	C12H10O4	018234-46-3	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052717\
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Acq On : 28 May 2017 4:14
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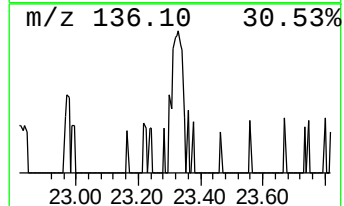
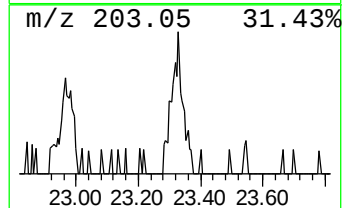
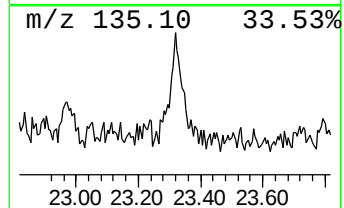
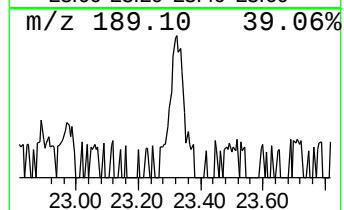
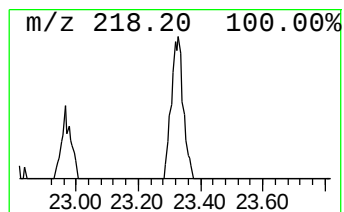
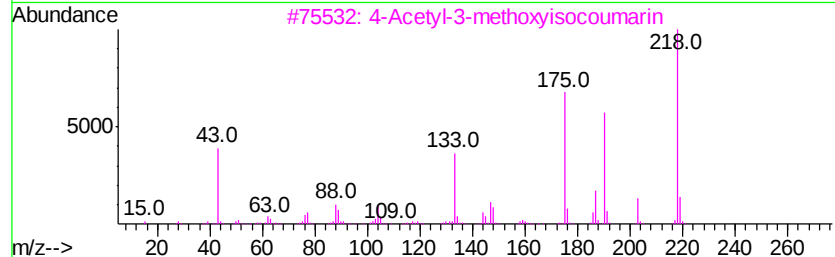
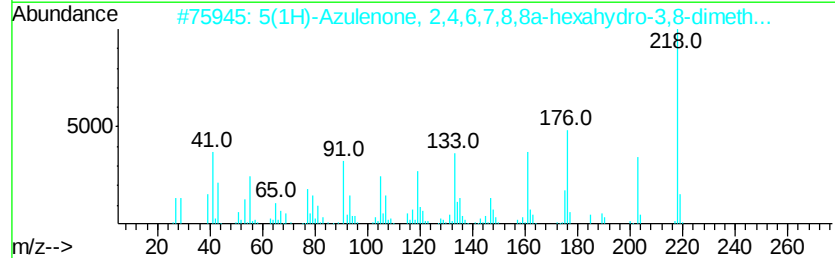
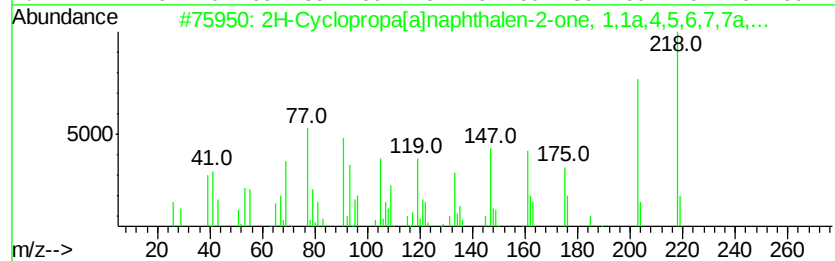
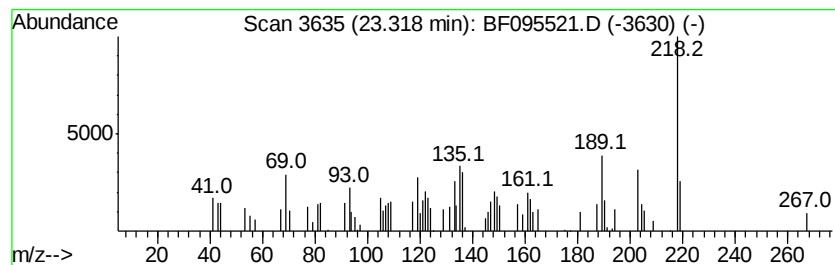
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown22.32 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.32	3.75 ng	88344	Perylene-d12	20.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2H-Cyclopropa[<i>a</i>]naphthalen-2-one...	218	C15H22O	006831-17-0	46
2		5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	43
3		4-Acetyl-3-methoxyisocoumarin	218	C12H10O4	003155-98-4	38
4		2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	35
5		Benzenamine, 2-bromo-4-nitro-	216	C6H5BrN2O2	013296-94-1	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052717\
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 NM5-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.10	9.1 ng		242962	1	7.74	534549	20.0
unknown7.40	7.40	88.1 ng		2354580	1	7.74	534549	20.0
Hexadecane	14.19	2.1 ng		48455	4	15.00	467017	20.0
Pentafluoropropio...	15.49	2.3 ng		54183	4	15.00	467017	20.0
6H-Cyclobuta[jk]p...	15.95	4.3 ng		99581	4	15.00	467017	20.0
1-Dodecanol, 2-oc...	18.55	3.6 ng		129849	5	18.67	714002	20.0
unknown20.07	20.07	3.2 ng		75459	6	20.35	470987	20.0
Hexacosane	20.79	2.9 ng		68047	6	20.35	470987	20.0
unknown21.86	21.86	3.2 ng		74799	6	20.35	470987	20.0
unknown22.97	22.97	2.8 ng		66212	6	20.35	470987	20.0
unknown22.32	23.32	3.8 ng		88344	6	20.35	470987	20.0