

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010419\
 Data File : BF111850.D
 Acq On : 4 Jan 2019 17:46
 Operator : JU/SJ
 Sample : K1017-25
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

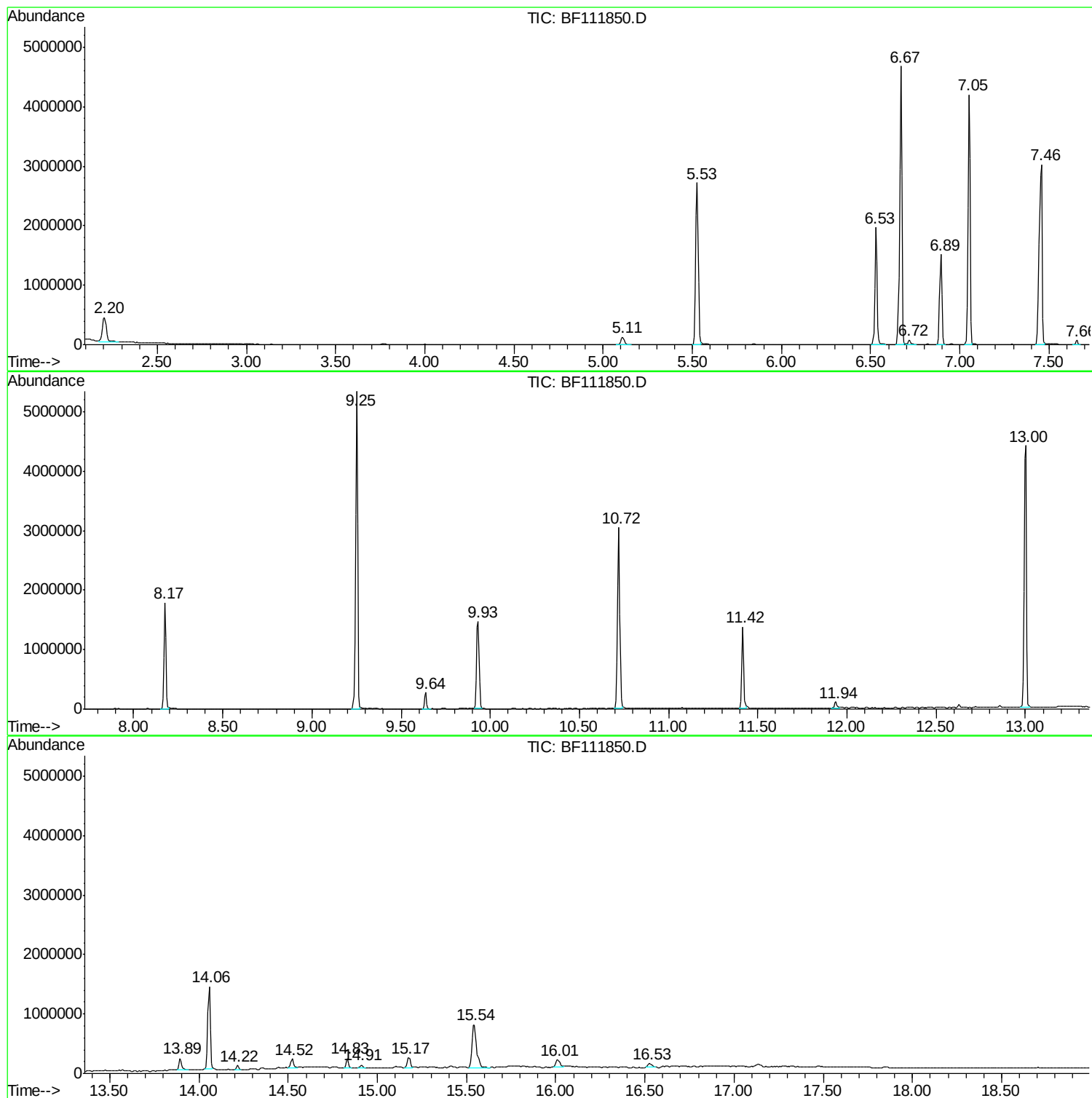
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	14	20	33	rVB	411486	599455	12.76%	1.616%
2	5.110	507	514	522	rBV	128575	155662	3.31%	0.420%
3	5.528	580	585	588	rBV	2716019	2507412	53.38%	6.758%
4	6.528	751	755	764	rBV	1966238	1753170	37.33%	4.725%
5	6.669	774	779	782	rBV	4676837	4270421	90.92%	11.510%
6	6.716	784	787	793	rVB	80336	79643	1.70%	0.215%
7	6.893	813	817	821	rBV	1513602	1183778	25.20%	3.191%
8	7.051	840	844	847	rBV	4198576	3783501	80.55%	10.198%
9	7.457	907	913	916	rBV	3020623	3173384	67.56%	8.553%
10	7.657	943	947	950	rVB	71249	59967	1.28%	0.162%
11	8.175	1031	1035	1039	rBV	1784252	1515644	32.27%	4.085%
12	9.251	1213	1218	1221	rBV	5338750	4697032	100.00%	12.660%
13	9.639	1280	1284	1288	rBV	271020	222601	4.74%	0.600%
14	9.934	1330	1334	1337	rBV	1455790	1359548	28.94%	3.664%
15	10.722	1463	1468	1471	rBV	3039438	2755147	58.66%	7.426%
16	11.416	1582	1586	1589	rBV	1372320	1121955	23.89%	3.024%
17	11.939	1670	1675	1678	rBV2	104305	109278	2.33%	0.295%
18	13.004	1851	1856	1859	rBV	4400409	4242627	90.33%	11.435%
19	13.892	2004	2007	2015	rBV	192540	218436	4.65%	0.589%
20	14.057	2031	2035	2038	rBV	1378746	1185504	25.24%	3.195%
21	14.216	2059	2062	2065	rBV	74302	63749	1.36%	0.172%
22	14.521	2110	2114	2119	rBV	148747	145354	3.09%	0.392%
23	14.833	2163	2167	2170	rVB	163204	161015	3.43%	0.434%
24	14.910	2177	2180	2184	rVB	53540	55570	1.18%	0.150%
25	15.174	2221	2225	2229	rBV	162489	183637	3.91%	0.495%
26	15.539	2282	2287	2303	rVB	722583	1214891	25.87%	3.275%
27	16.010	2363	2367	2373	rBV	118182	177053	3.77%	0.477%
28	16.527	2451	2455	2460	rVB2	63451	105356	2.24%	0.284%

Sum of corrected areas: 37100790

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



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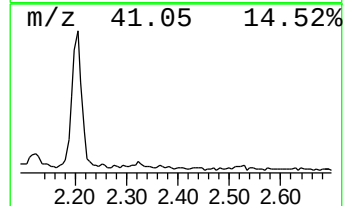
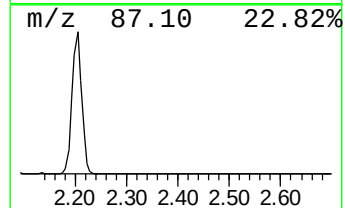
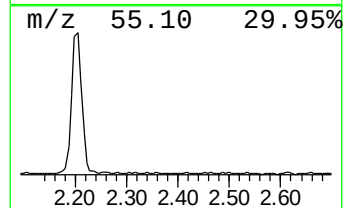
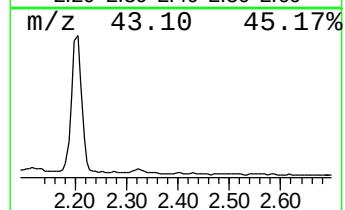
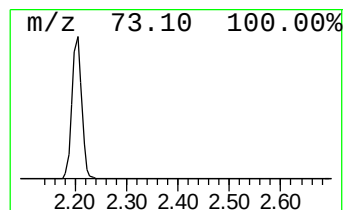
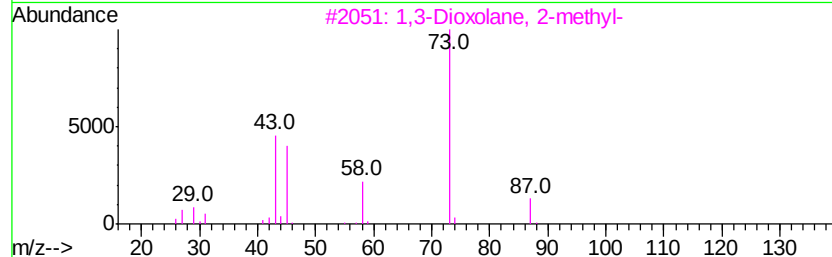
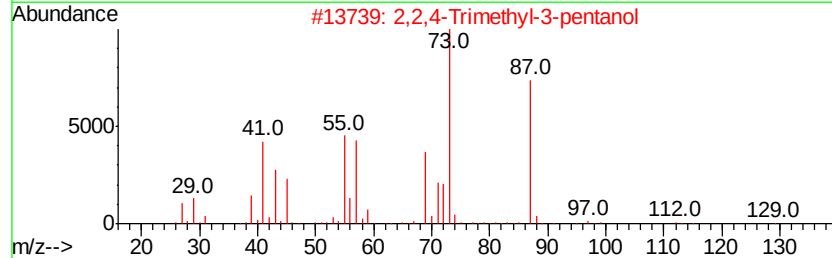
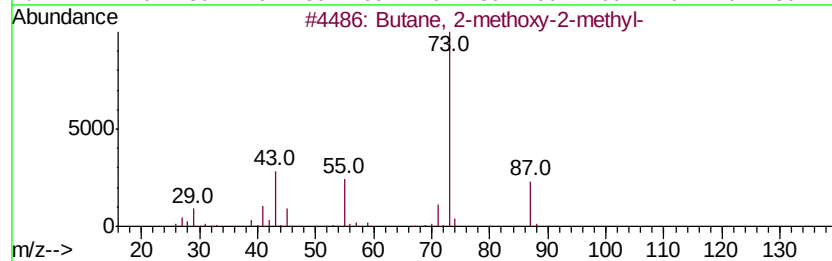
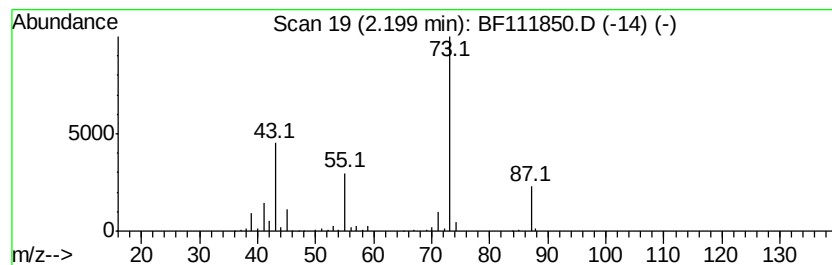
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	10.13 ng	599455	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	17
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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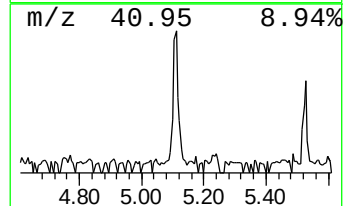
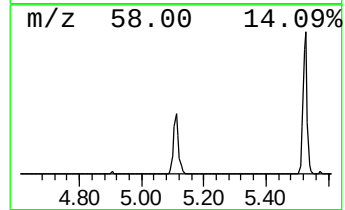
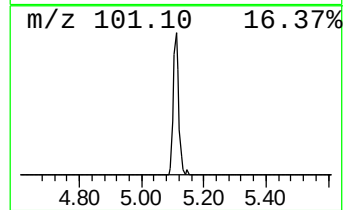
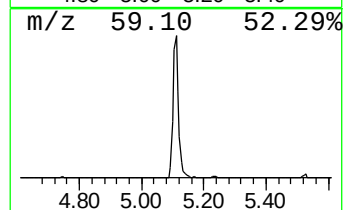
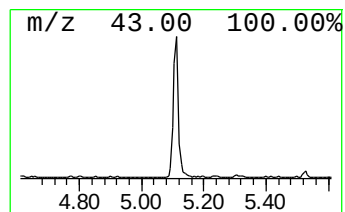
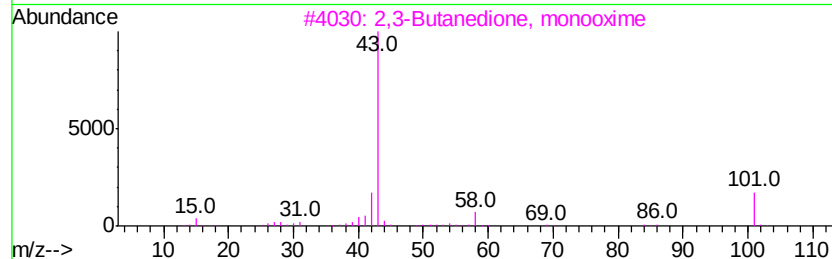
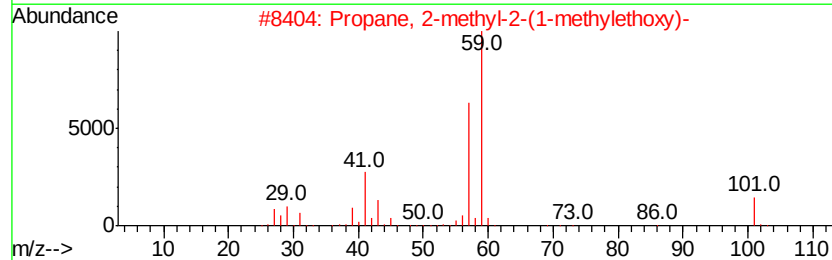
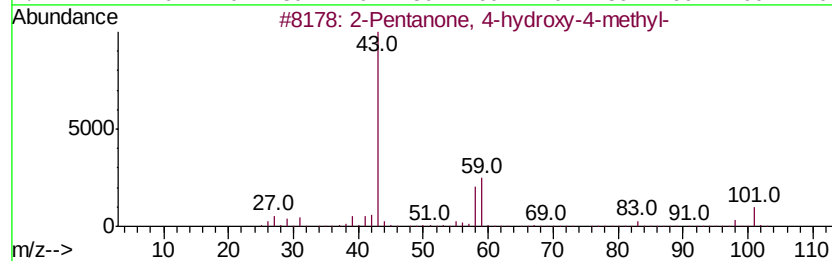
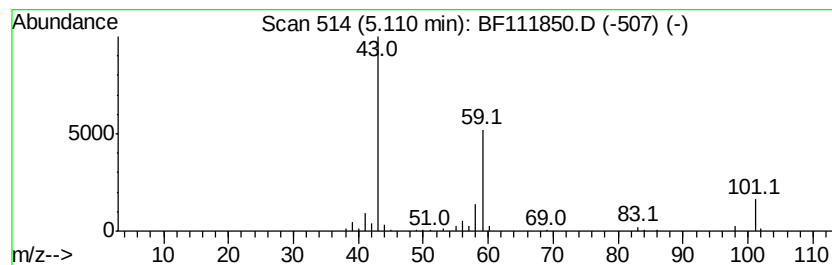
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	2.63 ng	155662	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	30
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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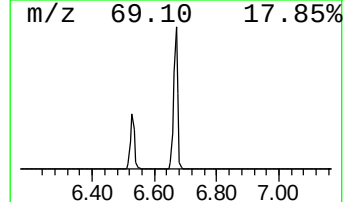
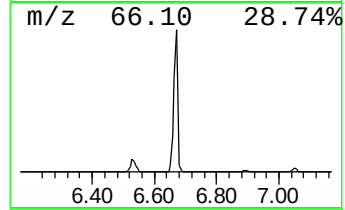
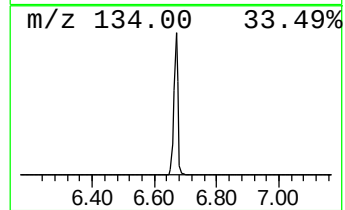
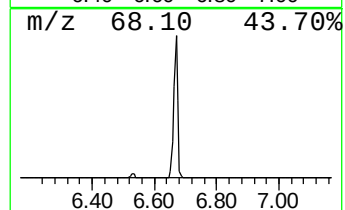
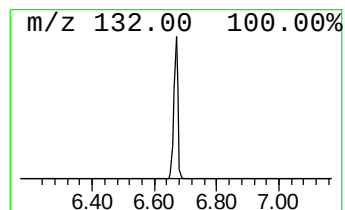
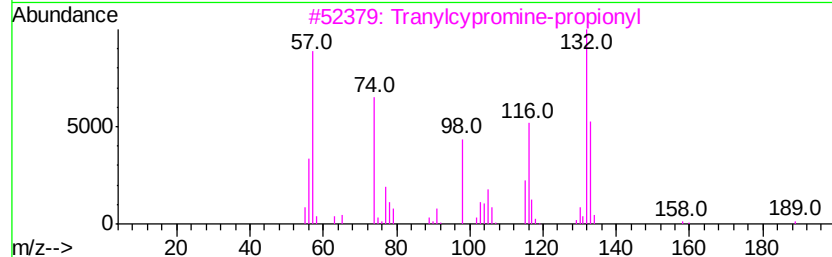
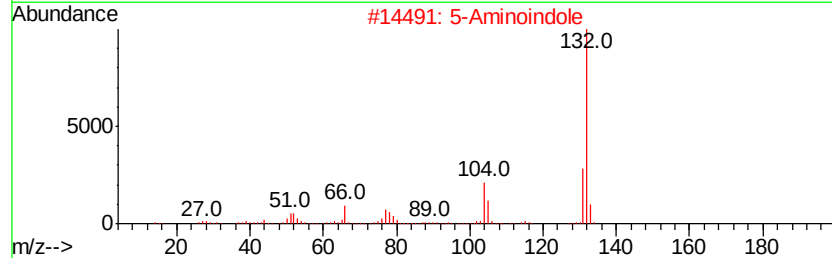
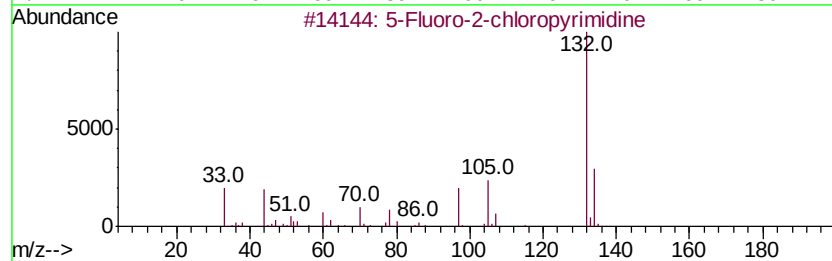
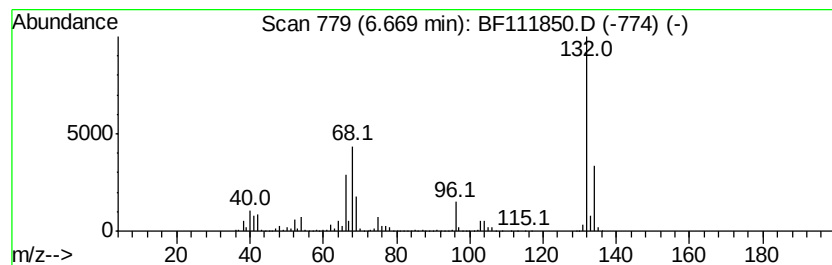
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Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	72.15 ng	4270420	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcyppromine-propionyl	189	C12H15NO	1000123-86-3	10
4			1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5			Xenon	132	Xe	007440-63-3	9



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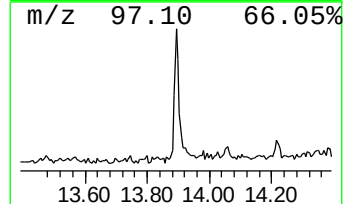
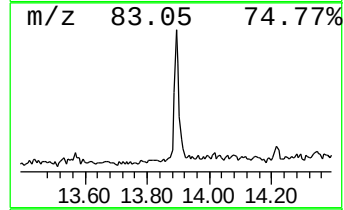
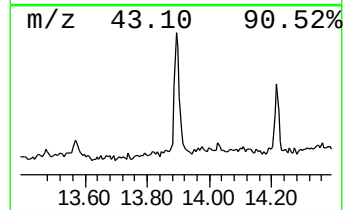
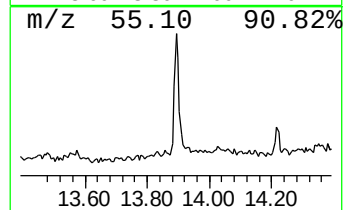
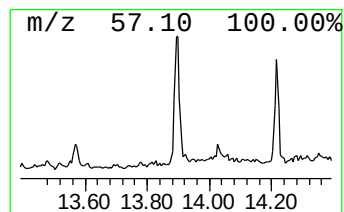
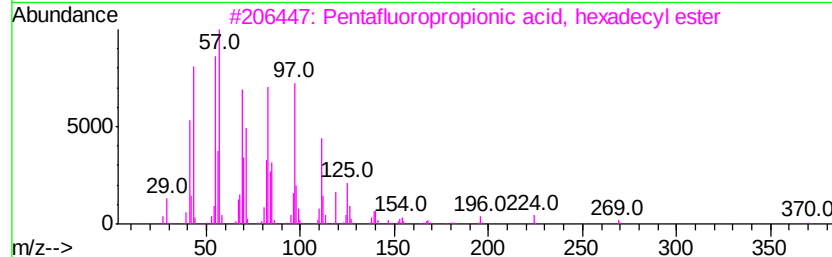
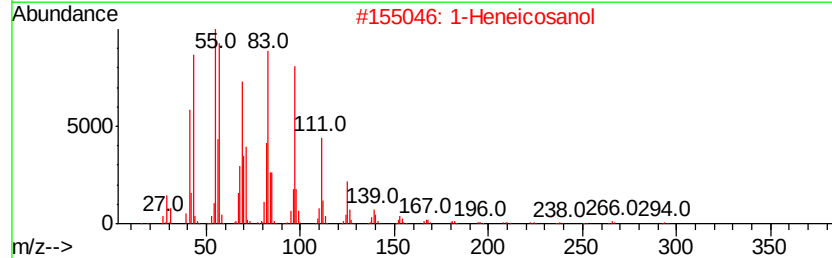
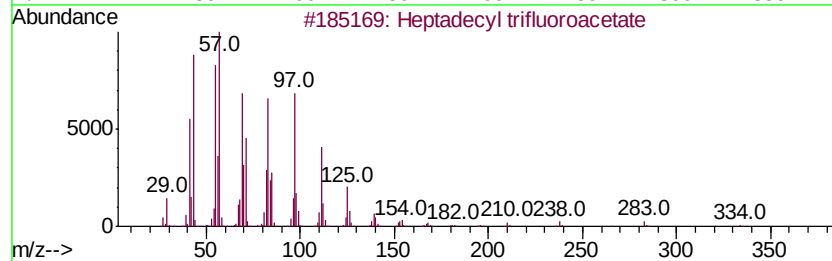
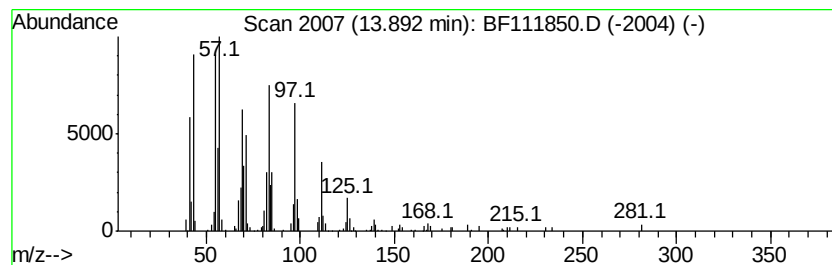
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Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	3.69 ng	218436	Chrysene-d12	14.06

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
2			1-Heneicosanol	312	C21H44O	015594-90-8	93
3			Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	91
4			Octacosanol	410	C28H58O	000557-61-9	91
5			Pentafluoropropionic acid, pentafluoropropyl ester	374	C18H31F5O2	959092-08-1	91



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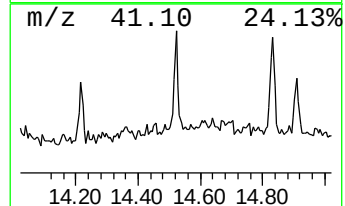
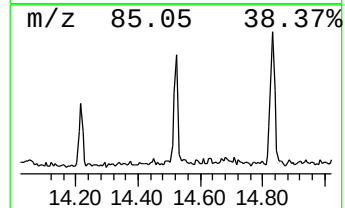
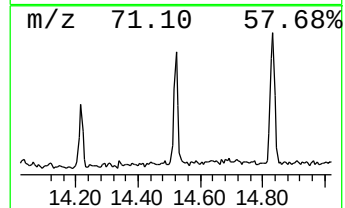
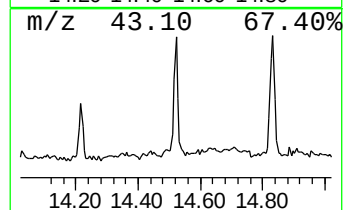
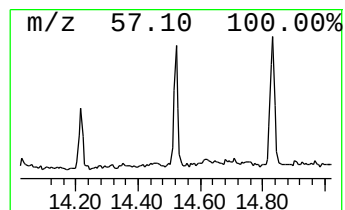
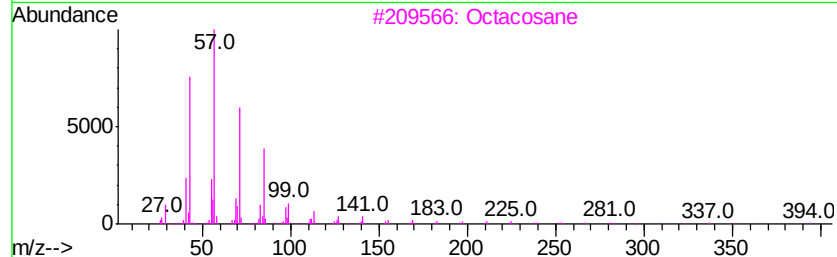
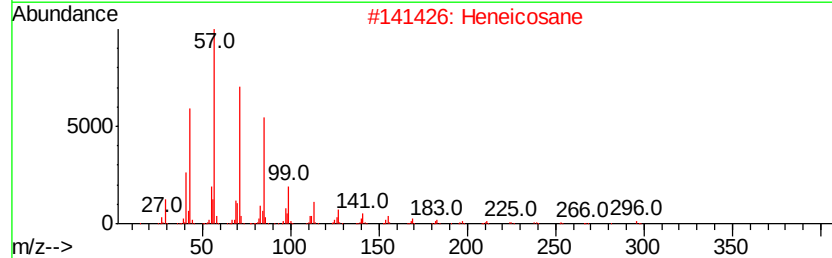
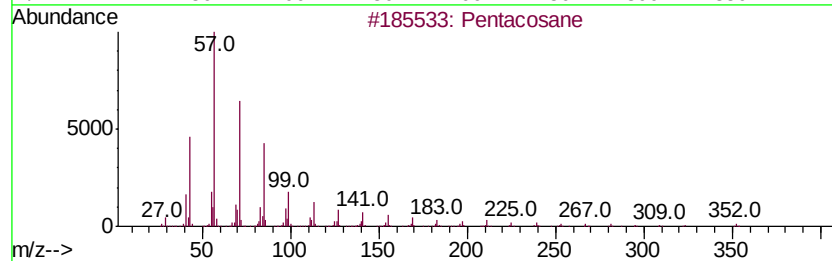
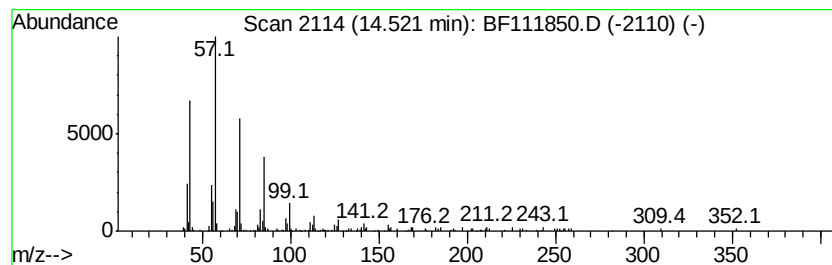
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Pentacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	2.45 ng	145354	Chrysene-d12	14.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane		352	C25H52	000629-99-2	90
2	Heneicosane		296	C21H44	000629-94-7	87
3	Octacosane		394	C28H58	000630-02-4	87
4	Tetracosane		338	C24H50	000646-31-1	87
5	Eicosane		282	C20H42	000112-95-8	87



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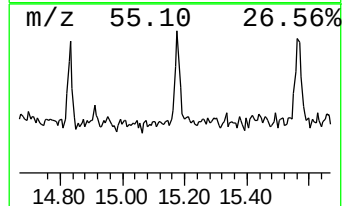
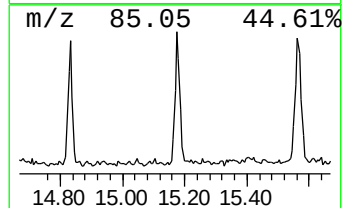
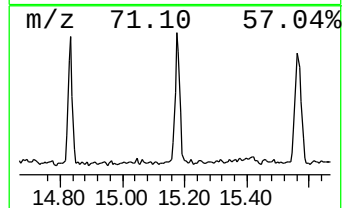
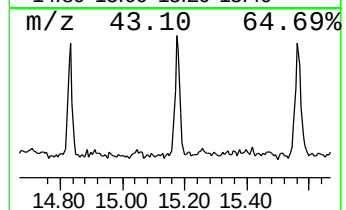
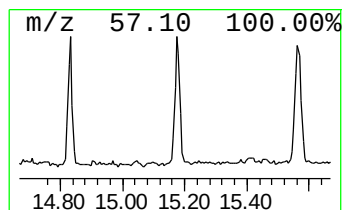
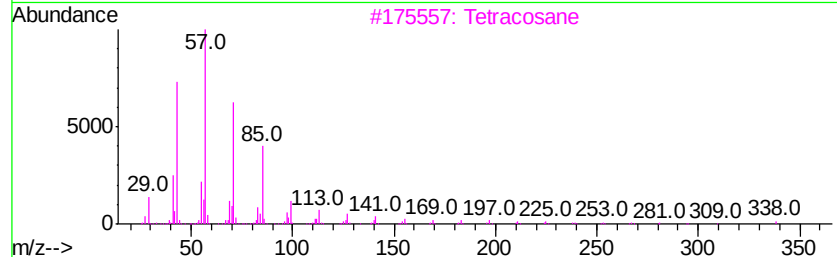
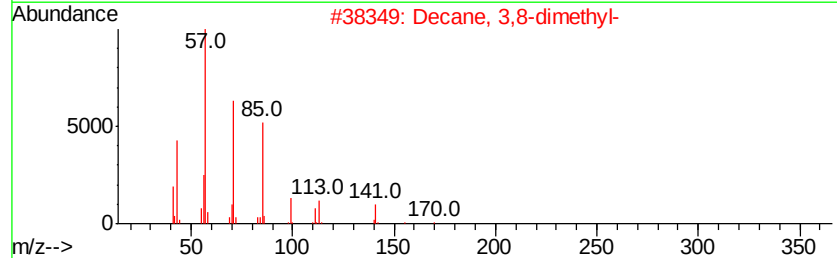
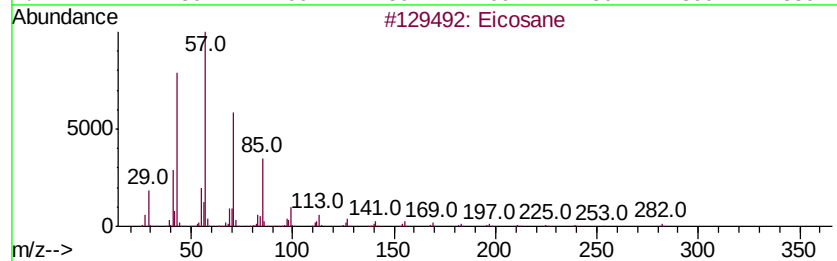
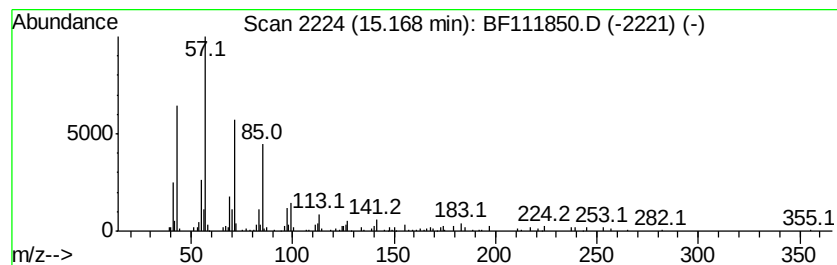
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	3.02 ng	183637	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	93
2		Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	91
3		Tetracosane	338	C24H50	000646-31-1	87
4		Heptacosane	380	C27H56	000593-49-7	87
5		Hexacosane	366	C26H54	000630-01-3	87



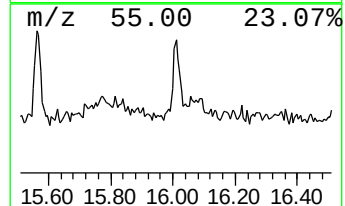
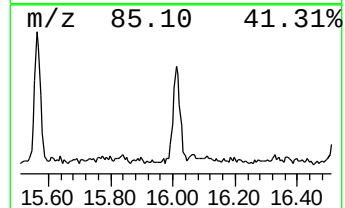
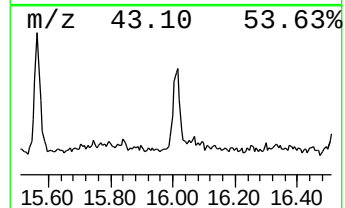
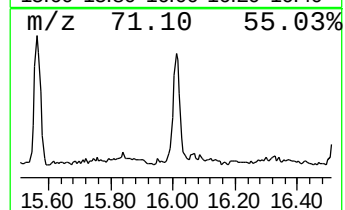
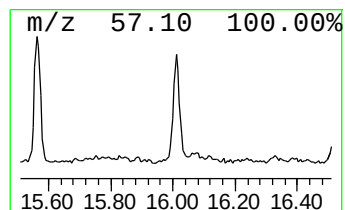
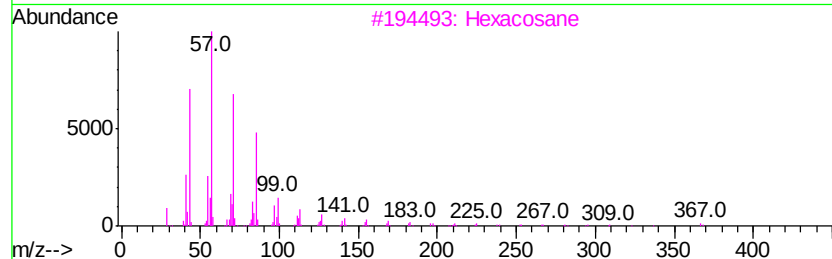
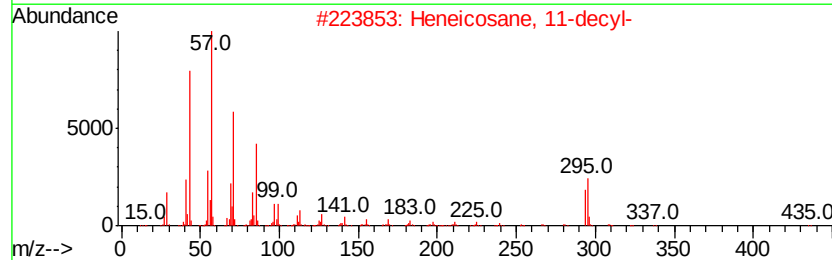
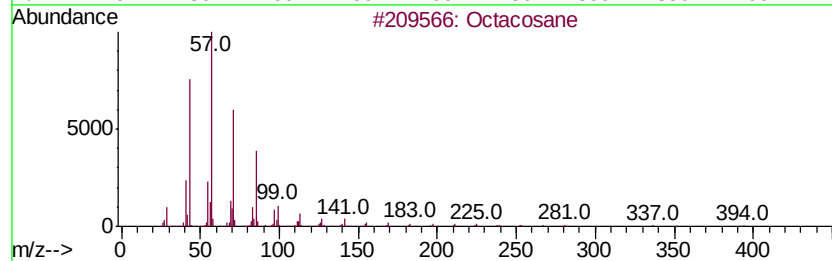
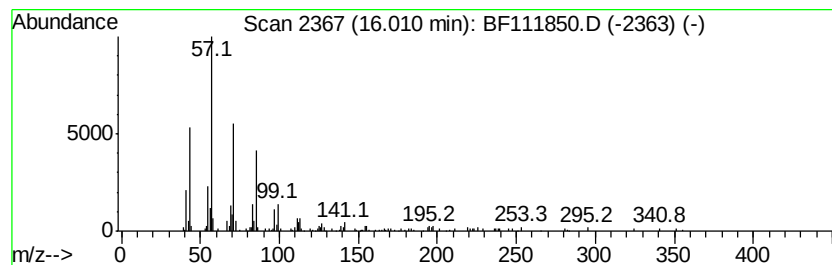
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Acq On : 4 Jan 2019 17:46
Operator : JU/SJ
Sample : K1017-25
Misc :
ALS Vial : 10 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.01	2.91 ng	177053	Perylene-d12	15.54	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Tricosane	324	C23H48	000638-67-5	87
5	Heptacosane	380	C27H56	000593-49-7	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF010419\
Data File : BF111850.D
Acq On : 4 Jan 2019 17:46
Operator : JU/SJ
Sample : K1017-25
Misc :
ALS Vial : 10 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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	10.1	ng	599455	1	6.89	1183780	20.0
2-Pentanone, 4-hy...	5.11	2.6	ng	155662	1	6.89	1183780	20.0
unknown6.67	6.67	72.2	ng	4270420	1	6.89	1183780	20.0
Heptadecyl triflu...	13.89	3.7	ng	218436	5	14.06	1185500	20.0
Pentacosane	14.52	2.5	ng	145354	5	14.06	1185500	20.0
Eicosane	15.17	3.0	ng	183637	6	15.54	1214890	20.0
Octacosane	16.01	2.9	ng	177053	6	15.54	1214890	20.0