

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
 Data File : BF102310.D
 Acq On : 22 Jan 2018 20:16
 Operator : SJ/JU
 Sample : J1116-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-41-4.5-5.0

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-BF012218.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	4.916	476	481	493	rBV	168781	246758	7.08%	0.809%
2	5.328	546	551	554	rBV	3247953	3317227	95.17%	10.878%
3	6.357	720	726	743	rBV	2954867	3485403	100.00%	11.430%
4	6.487	743	748	751	rBV	3591027	3410865	97.86%	11.185%
5	6.716	783	787	794	rBV	843394	798473	22.91%	2.618%
6	6.869	809	813	816	rBV	2758855	2428195	69.67%	7.963%
7	7.281	878	883	886	rBV	2130776	2127981	61.05%	6.978%
8	7.992	1000	1004	1018	rBV	1106708	1087198	31.19%	3.565%
9	9.075	1182	1188	1191	rBV	3399800	3091841	88.71%	10.139%
10	9.469	1251	1255	1258	rBV	502556	428633	12.30%	1.406%
11	9.681	1287	1291	1294	rBV	136568	107142	3.07%	0.351%
12	9.745	1299	1302	1308	rVB	1174653	1107297	31.77%	3.631%
13	10.180	1372	1376	1379	rVB	153958	131830	3.78%	0.432%
14	10.398	1408	1413	1415	rBV	43924	51309	1.47%	0.168%
15	10.539	1430	1437	1440	rBV	2139470	2026594	58.15%	6.646%
16	10.651	1453	1456	1465	rVB	137729	137309	3.94%	0.450%
17	11.098	1529	1532	1535	rBV	52644	44285	1.27%	0.145%
18	11.233	1551	1555	1558	rBV	1127875	1010200	28.98%	3.313%
19	12.639	1791	1794	1797	rBV	144121	110396	3.17%	0.362%
20	12.816	1820	1824	1828	rBV	2410356	2369988	68.00%	7.772%
21	13.345	1911	1914	1917	rBV	92303	77786	2.23%	0.255%
22	13.710	1972	1976	1983	rBV	591513	614364	17.63%	2.015%
23	13.868	1996	2003	2006	rBV2	860829	1055690	30.29%	3.462%
24	14.033	2028	2031	2037	rBV	36010	40729	1.17%	0.134%
25	14.345	2080	2084	2087	rBV4	55003	75051	2.15%	0.246%
26	14.704	2142	2145	2149	rVB	50452	47095	1.35%	0.154%
27	14.957	2184	2188	2190	rBV	46438	50987	1.46%	0.167%
28	15.292	2240	2245	2253	rBV	617733	808740	23.20%	2.652%
29	15.721	2315	2318	2322	rVB2	40898	45746	1.31%	0.150%
30	15.774	2322	2327	2333	rBV2	91869	159092	4.56%	0.522%

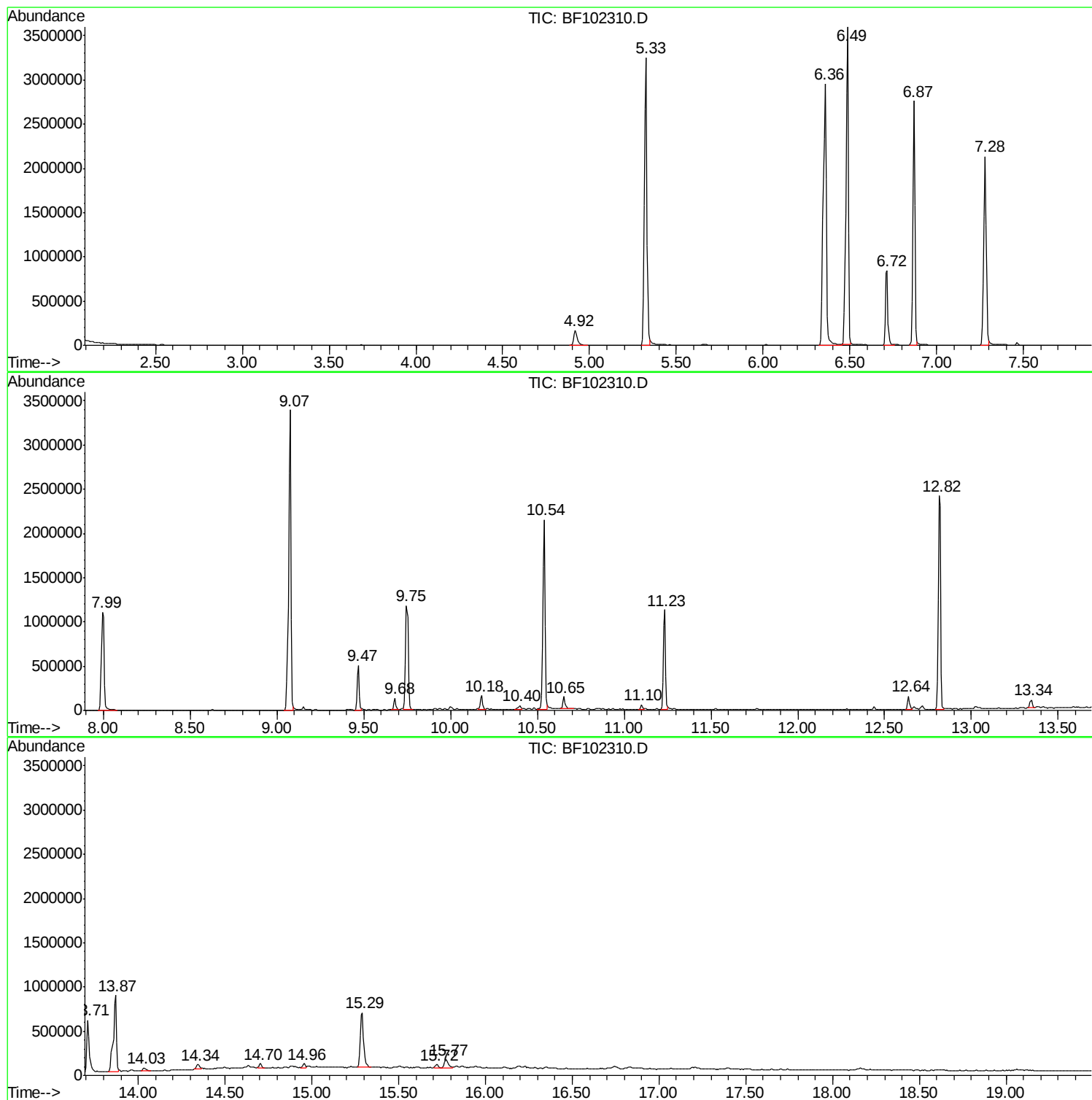
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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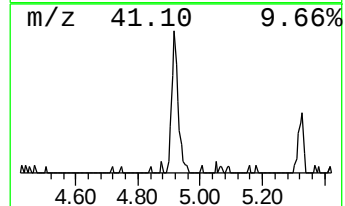
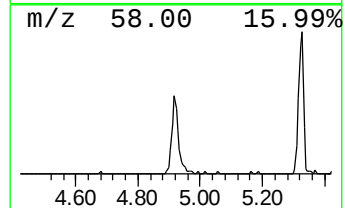
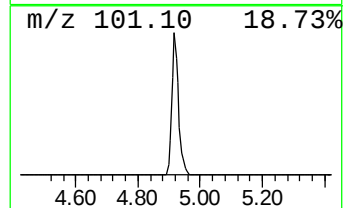
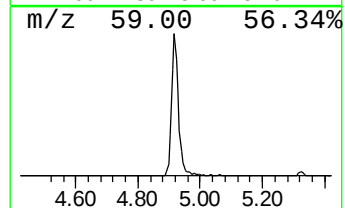
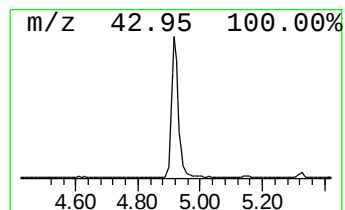
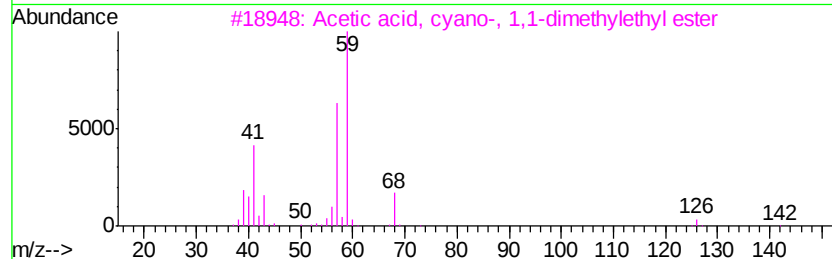
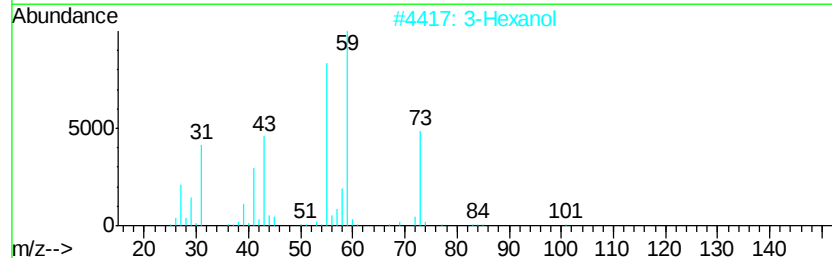
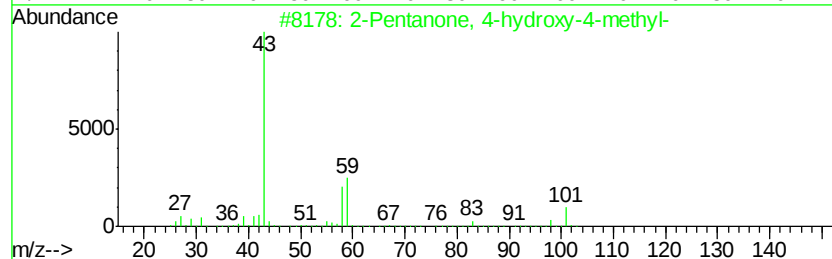
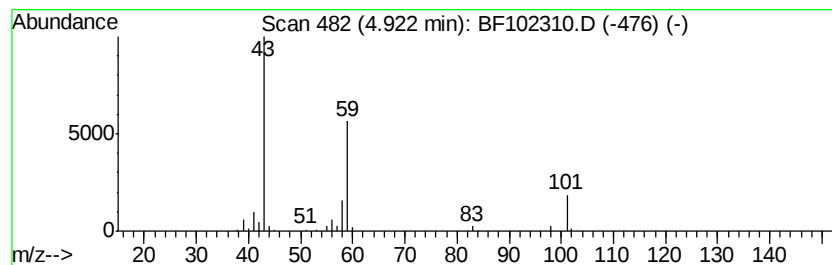
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	6.18 ng	246758	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		3-Hexanol	102	C6H14O	000623-37-0	33
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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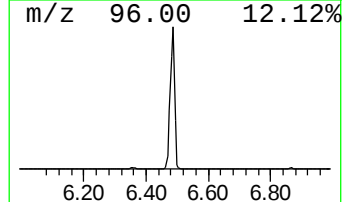
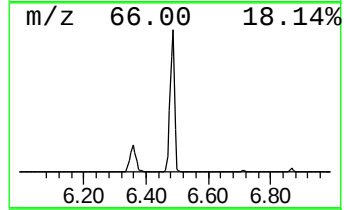
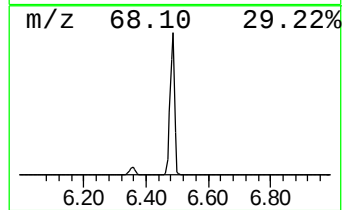
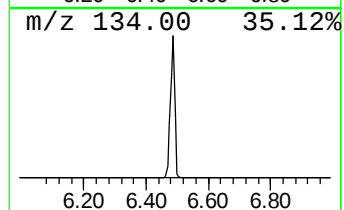
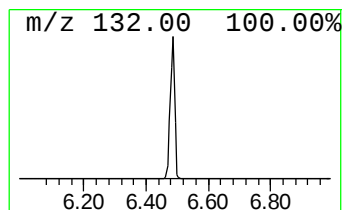
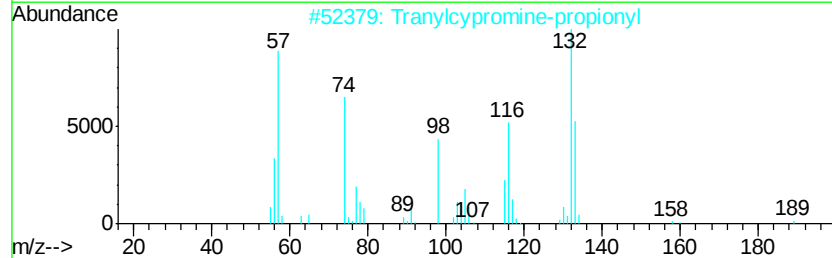
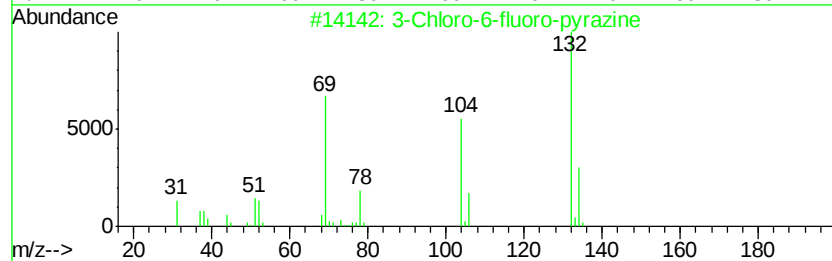
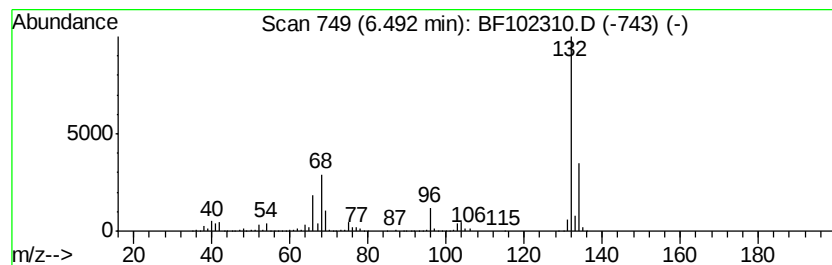
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	85.43 ng	3410870	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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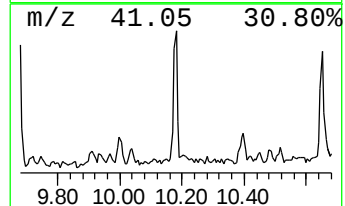
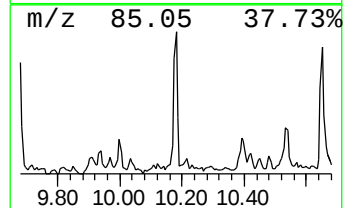
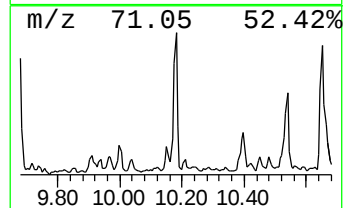
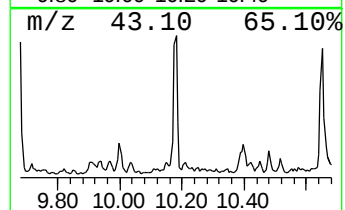
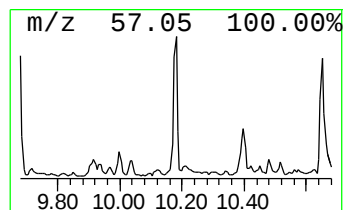
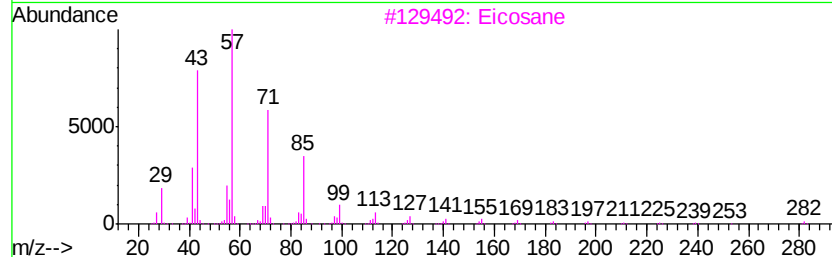
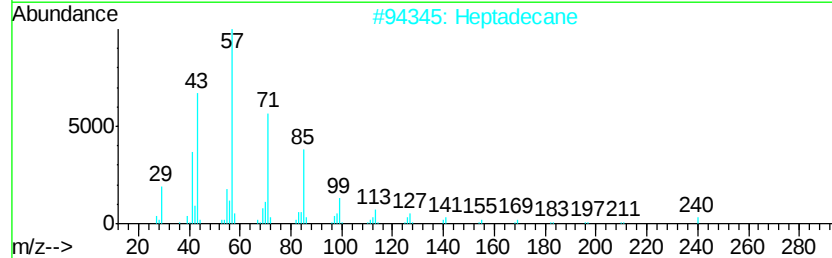
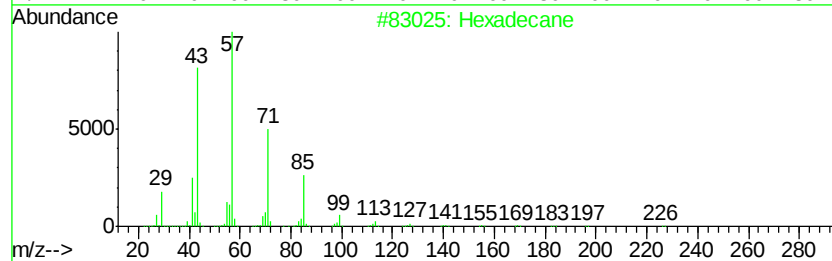
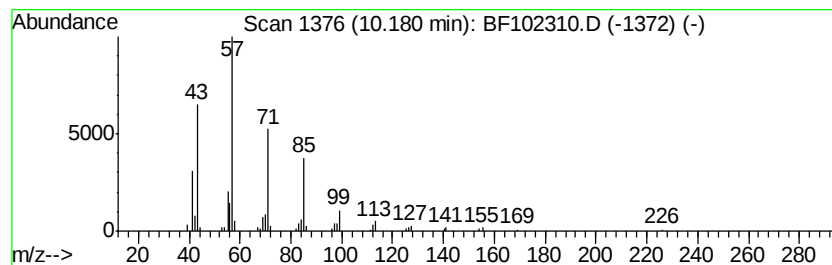
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Peak Number 4 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.18	2.38 ng	131830	Acenaphthene-d10	9.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	97
2	Heptadecane		240	C17H36	000629-78-7	90
3	Eicosane		282	C20H42	000112-95-8	90
4	Dodecane, 2-methyl-6-propyl-		226	C16H34	055045-08-4	86
5	Tetradecane		198	C14H30	000629-59-4	80



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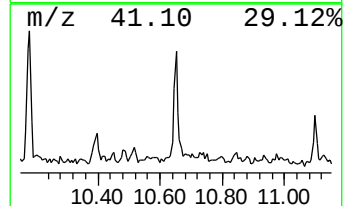
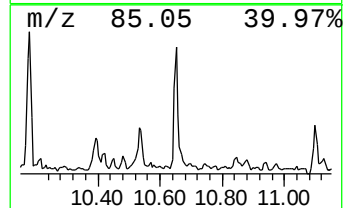
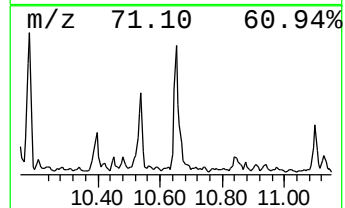
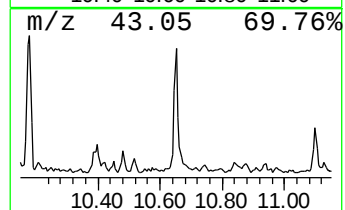
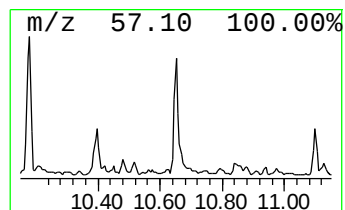
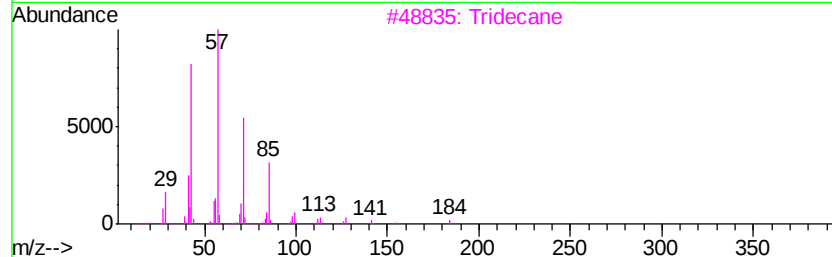
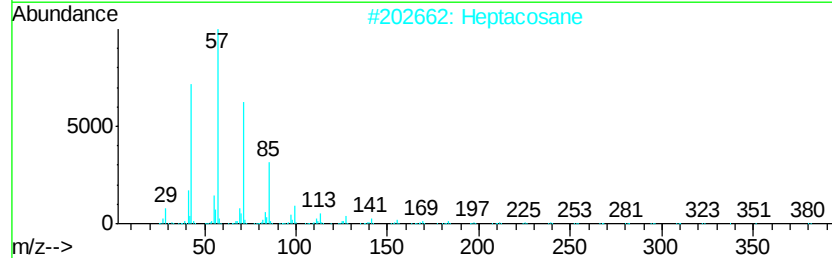
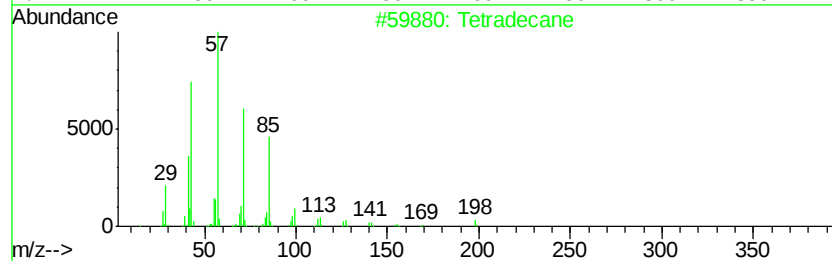
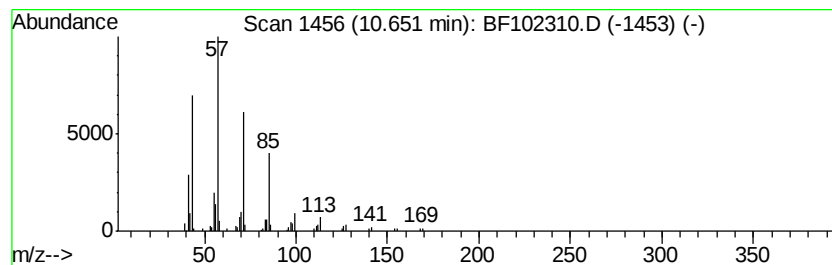
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	2.72 ng	137309	Phenanthrene-d10	11.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	91
2		Heptacosane	380	C27H56	000593-49-7	90
3		Tridecane	184	C13H28	000629-50-5	90
4		Hexadecane	226	C16H34	000544-76-3	90
5		Heneicosane	296	C21H44	000629-94-7	90



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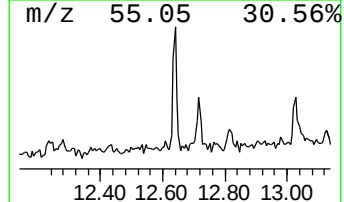
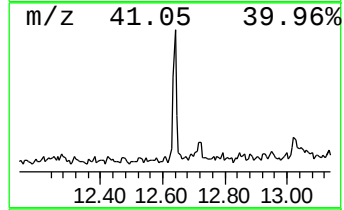
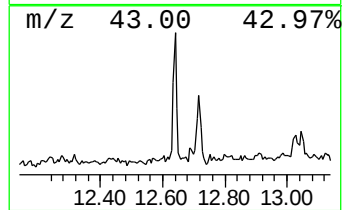
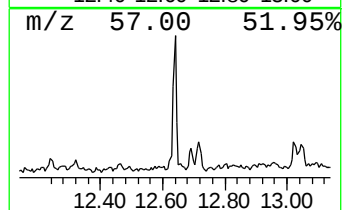
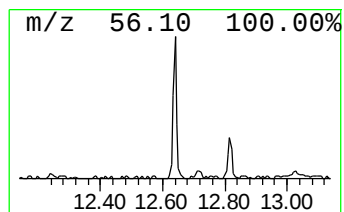
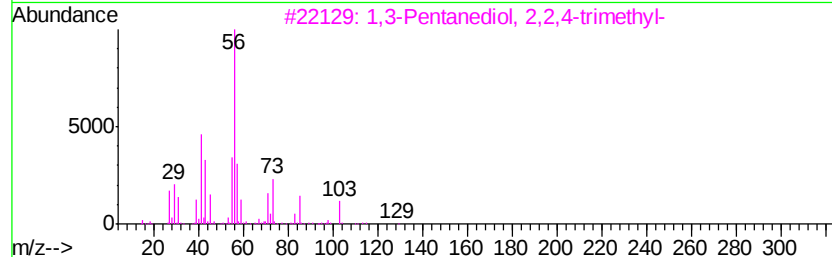
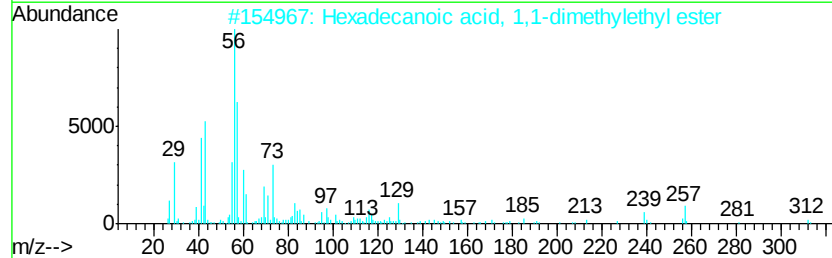
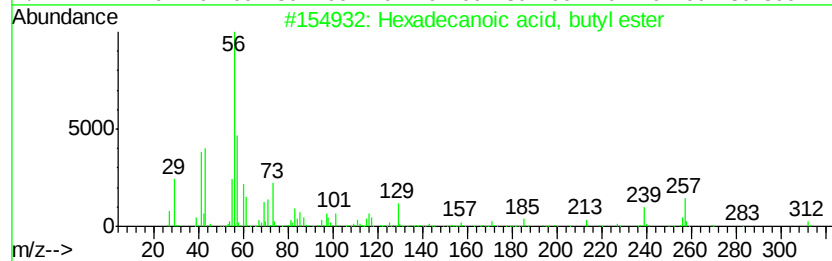
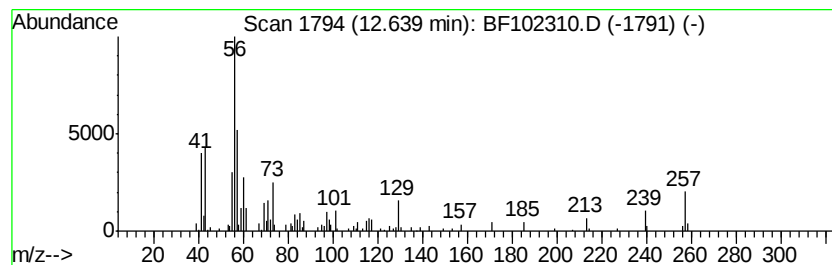
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	2.09 ng	110396	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	87
3		1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	43
4		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	38
5		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	38



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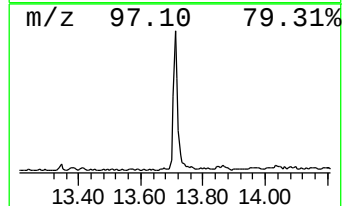
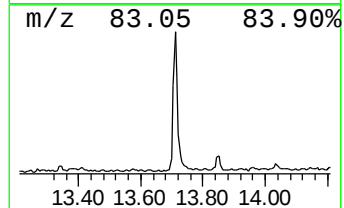
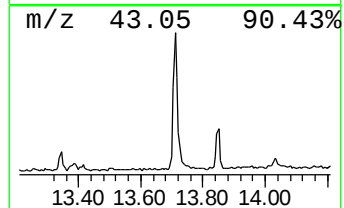
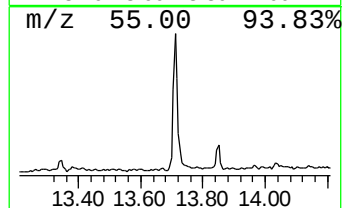
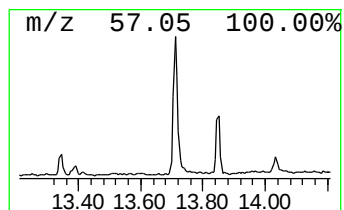
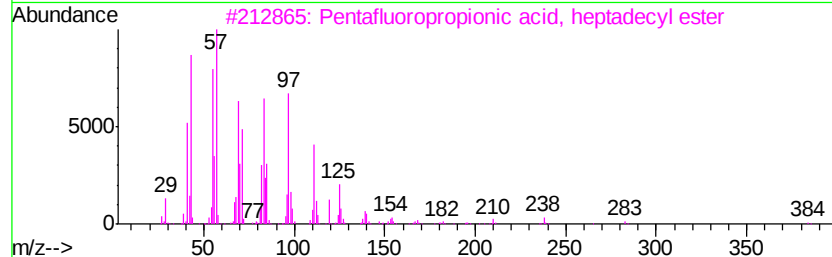
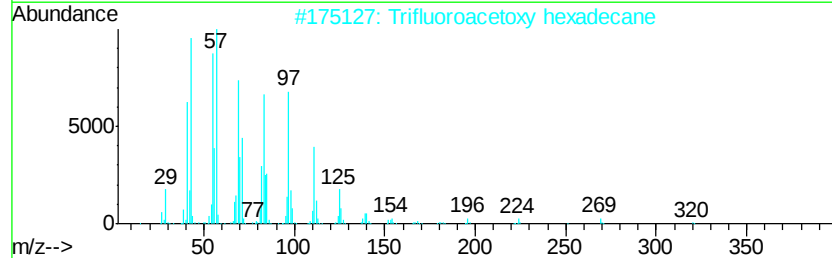
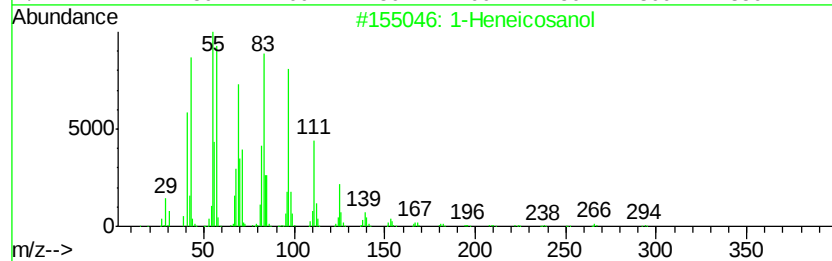
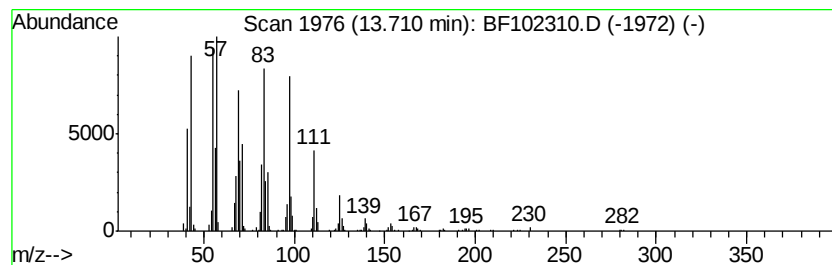
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	11.64 ng	614364	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol		312	C21H44O	015594-90-8	95
2	Trifluoroacetoxy hexadecane		338	C18H33F3O2	006222-03-3	94
3	Pentafluoropropionic acid, hepta...		402	C20H35F5O2	959218-78-1	94
4	Heptafluorobutyric acid, hexadec...		438	C20H33F7O2	006385-15-5	94
5	3-Eicosene, (E)-		280	C20H40	074685-33-9	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012218\
Data File : BF102310.D
Acq On : 22 Jan 2018 20:16
Operator : SJ/JU
Sample : J1116-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

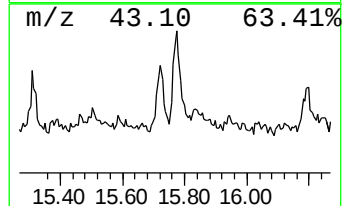
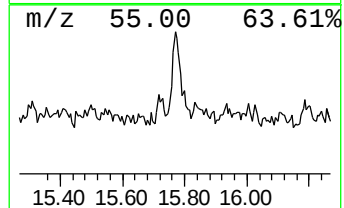
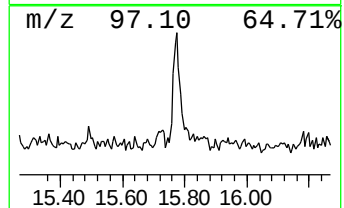
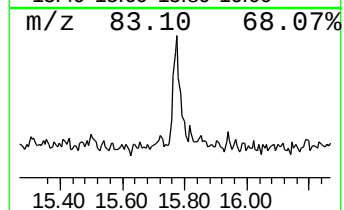
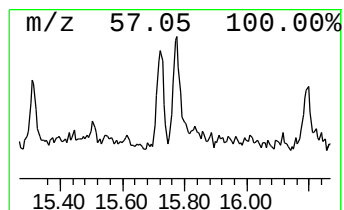
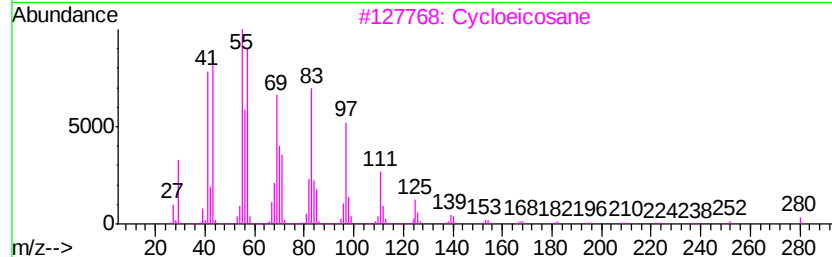
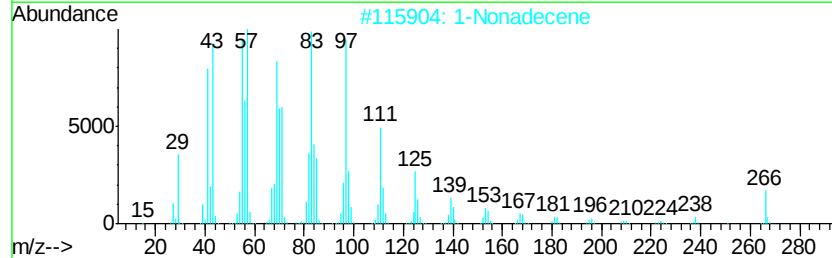
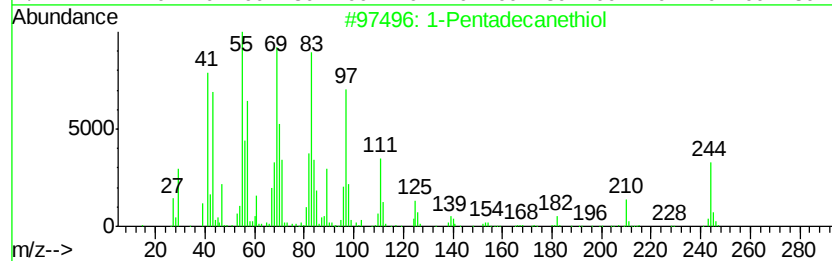
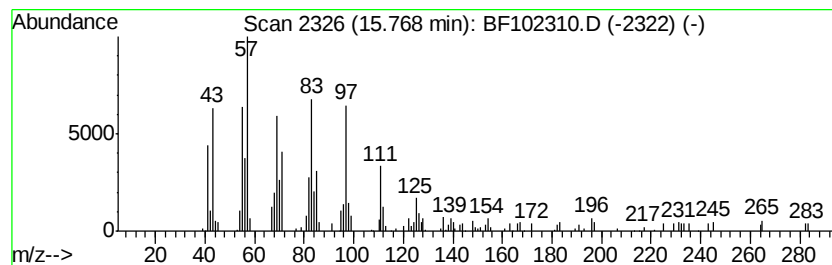
Instrument :
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ClientSampleId :
SB-41-4.5-5.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Pentadecanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.77	3.93 ng	159092	Perylene-d12		15.29	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentadecanethiol	244	C15H32S	025276-70-4	89
2		1-Nonadecene	266	C19H38	018435-45-5	83
3		Cvcloeicosane	280	C20H40	000296-56-0	80
4		Cyclotetradecane	196	C14H28	000295-17-0	70
5		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	62



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012218\
Data File : BF102310.D
Acq On : 22 Jan 2018 20:16
Operator : SJ/JU
Sample : J1116-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-41-4.5-5.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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...	4.92	6.2	ng	246758	1	6.72	798473	20.0
unknown6.49	6.49	85.4	ng	3410870	1	6.72	798473	20.0
Hexadecane	10.18	2.4	ng	131830	3	9.75	1107300	20.0
Tetradecane	10.65	2.7	ng	137309	4	11.23	1010200	20.0
Hexadecanoic acid...	12.64	2.1	ng	110396	5	13.87	1055690	20.0
1-Heneicosanol	13.71	11.6	ng	614364	5	13.87	1055690	20.0
1-Pentadecanethiol	15.77	3.9	ng	159092	6	15.29	808740	20.0