

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040518\
 Data File : BF104283.D
 Acq On : 5 Apr 2018 21:27
 Operator : JU/SJ
 Sample : J2237-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SC-1

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-BF032818.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	2.281	28	33	42	rVB	119276	164983	5.15%	0.654%
2	5.193	525	528	537	rBV	38664	70821	2.21%	0.281%
3	5.581	591	594	624	rBV	822894	2074077	64.75%	8.224%
4	6.581	761	764	784	rBV	1010282	2314020	72.24%	9.176%
5	6.716	784	787	820	rVV	1602747	2987030	93.26%	11.845%
6	6.951	824	827	848	rVV	159303	547152	17.08%	2.170%
7	7.098	848	852	876	rVB	1263819	1976422	61.70%	7.837%
8	7.516	919	923	945	rBV	556543	1471703	45.95%	5.836%
9	8.228	1040	1044	1061	rBV	360862	740966	23.13%	2.938%
10	9.292	1222	1225	1248	rBV	2169903	3203053	100.00%	12.701%
11	9.692	1286	1293	1304	rBV	92031	148826	4.65%	0.590%
12	9.980	1338	1342	1360	rBV	757144	954079	29.79%	3.783%
13	10.386	1408	1411	1414	rBV	56207	45842	1.43%	0.182%
14	10.775	1474	1477	1489	rBV	1225778	1909529	59.62%	7.572%
15	10.857	1489	1491	1503	rVB	91338	163592	5.11%	0.649%
16	11.480	1593	1597	1619	rBV	561934	1000491	31.24%	3.967%
17	11.980	1679	1682	1693	rBV3	41164	69601	2.17%	0.276%
18	12.933	1840	1844	1852	rVB2	37722	46800	1.46%	0.186%
19	13.063	1861	1866	1888	rBV	2423274	3167712	98.90%	12.561%
20	13.927	2010	2013	2029	rBV	265613	335769	10.48%	1.331%
21	14.133	2044	2048	2065	rBV	595224	929860	29.03%	3.687%
22	14.574	2115	2123	2127	rBV6	17401	37638	1.18%	0.149%
23	14.951	2183	2187	2192	rVB	145402	154996	4.84%	0.615%
24	15.662	2303	2308	2323	rBV	325225	655650	20.47%	2.600%
25	16.139	2384	2389	2398	rBV7	19100	47676	1.49%	0.189%

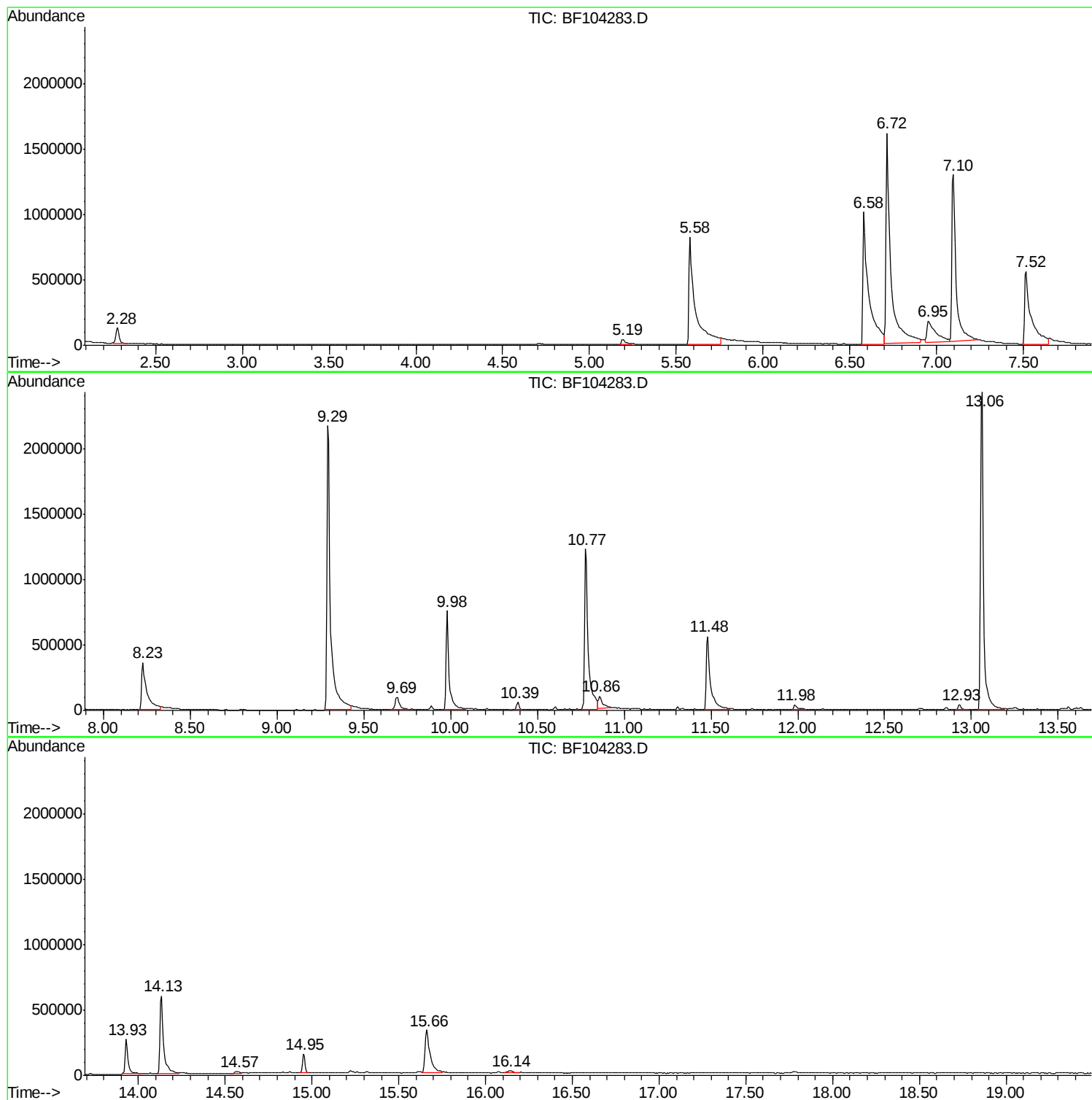
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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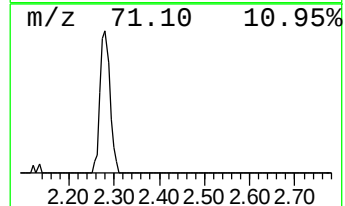
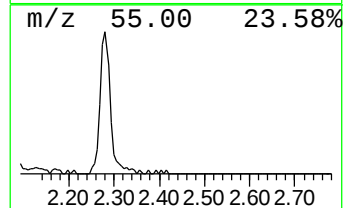
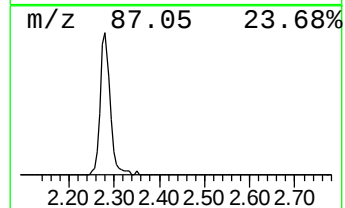
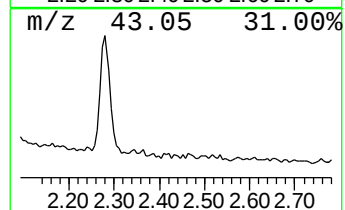
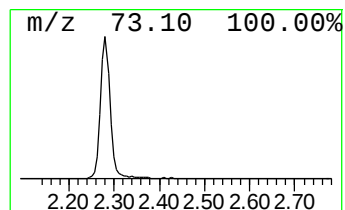
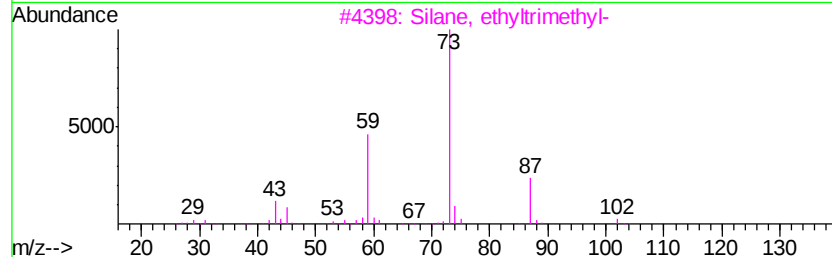
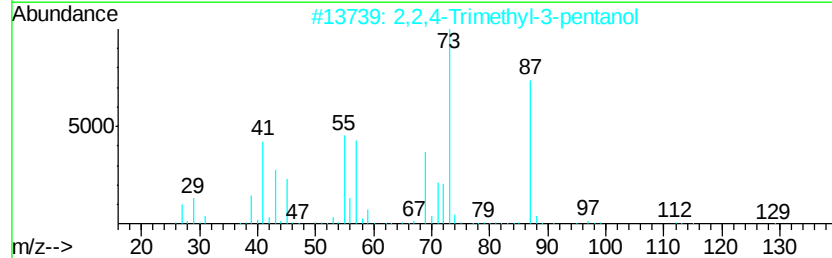
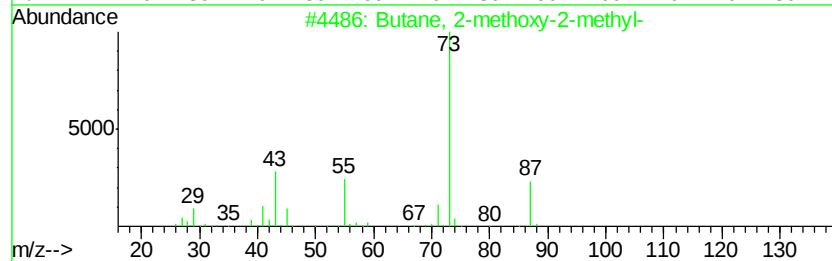
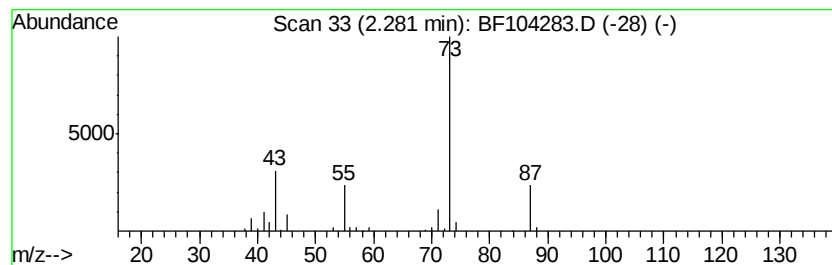
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.28	6.03 ng	164983	1,4-Dichlorobenzene-d4	6.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17



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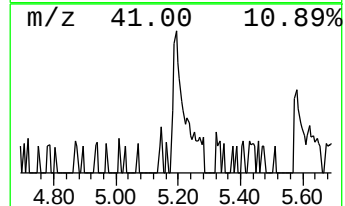
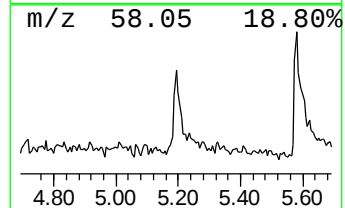
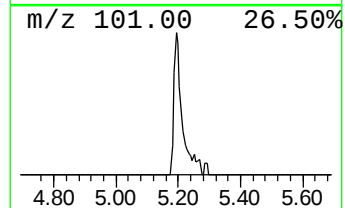
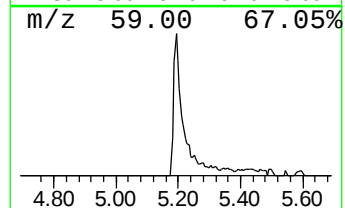
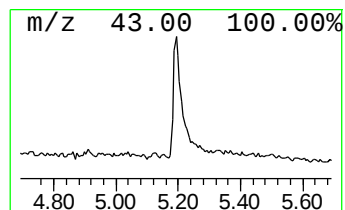
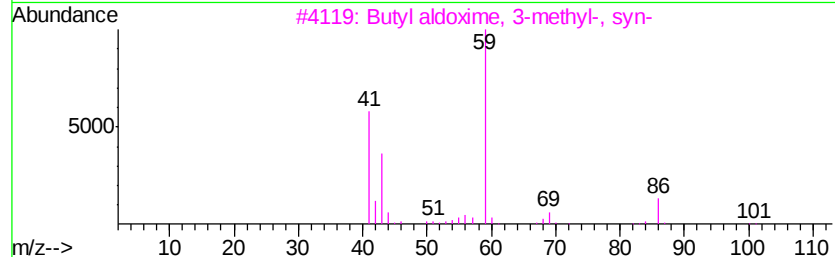
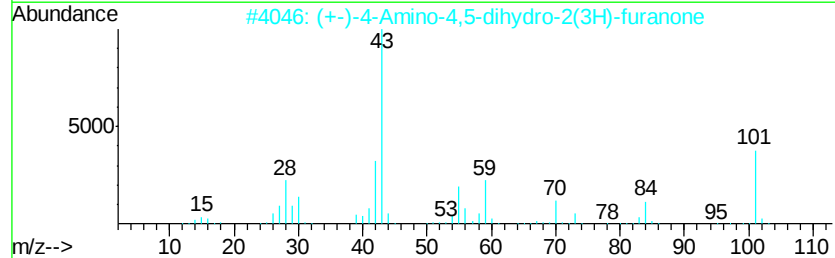
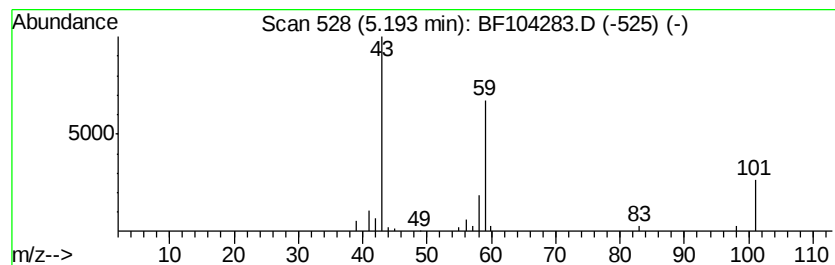
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	2.59 ng	70821	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	28
3		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
4		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
5		Acetone	58	C3H6O	000067-64-1	9



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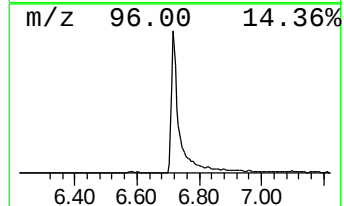
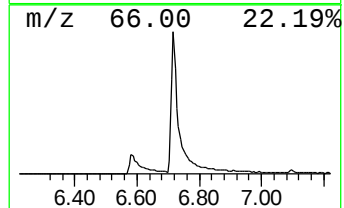
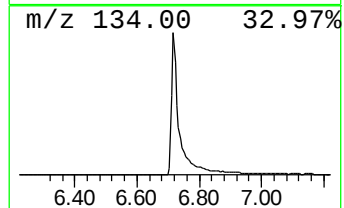
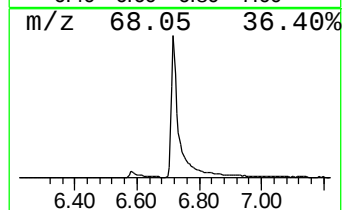
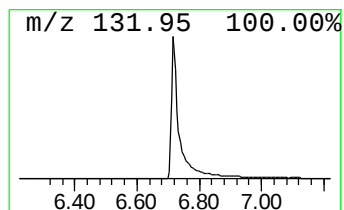
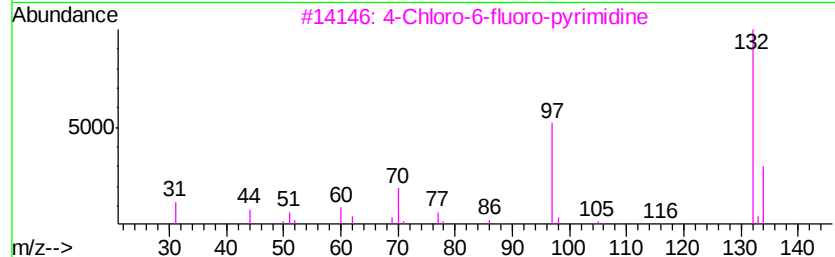
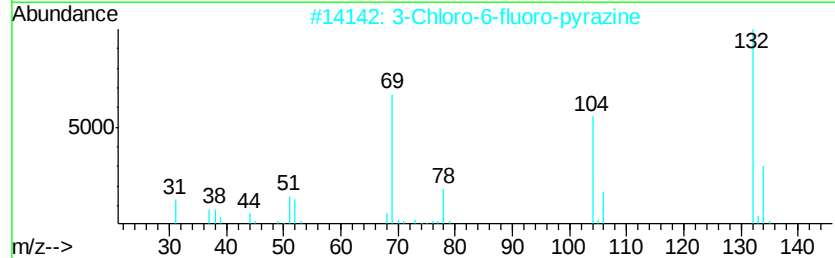
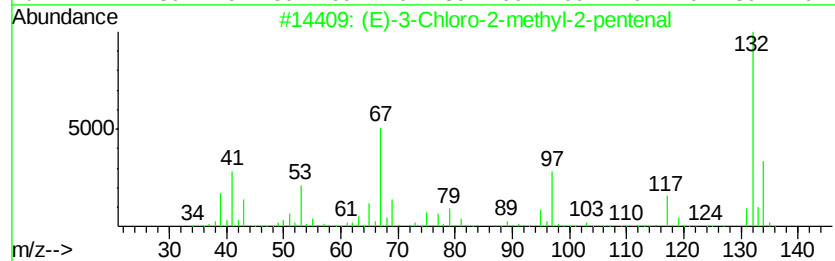
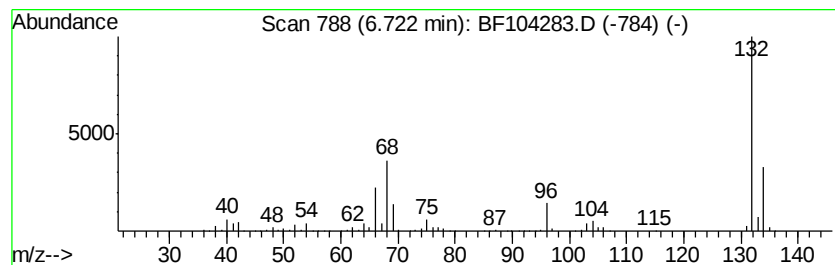
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Peak Number 3 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	109.19 ng	2987030	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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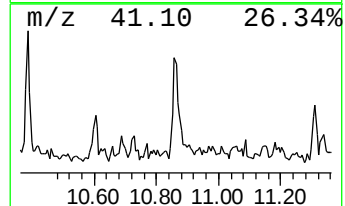
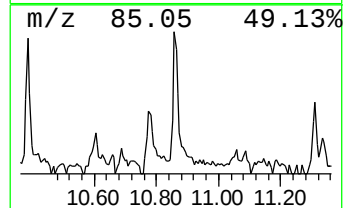
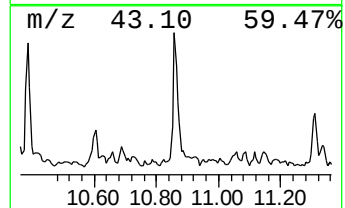
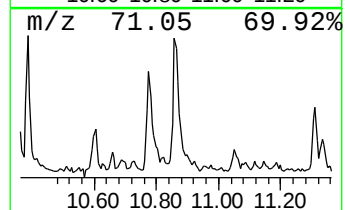
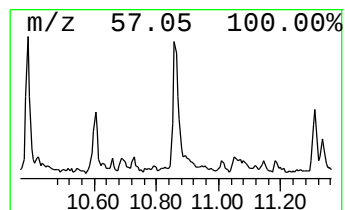
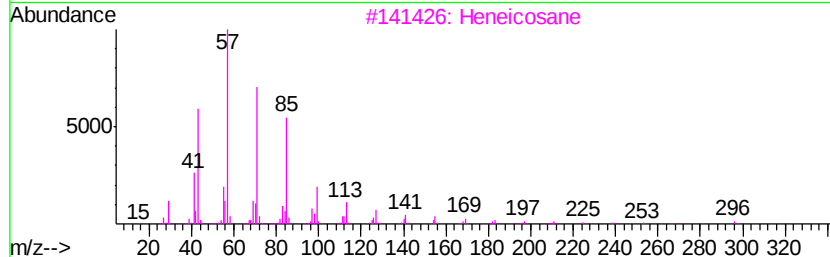
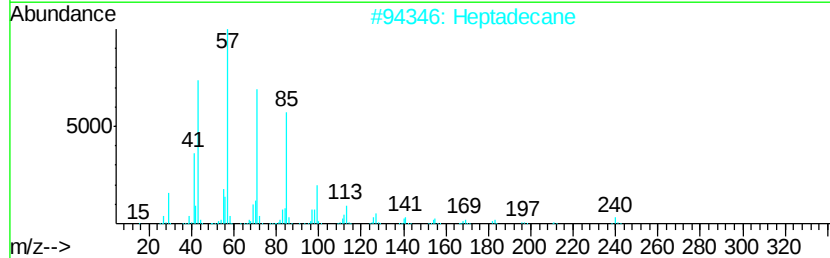
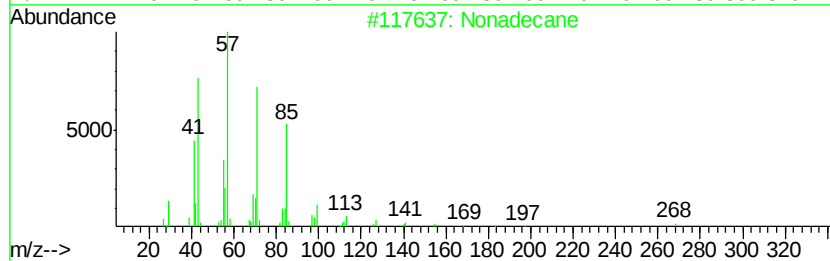
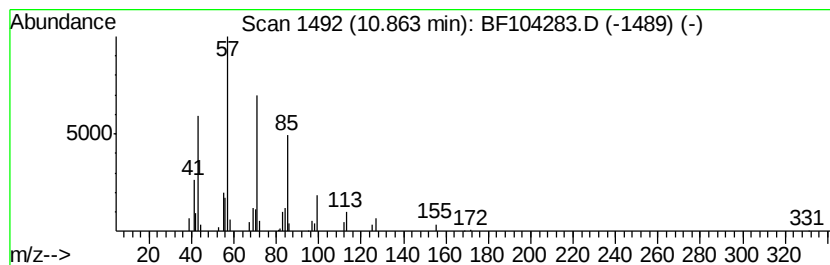
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.86	3.27 ng	163592	Phenanthrene-d10	11.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Heptadecane	240	C17H36	000629-78-7	90
3	Heneicosane	296	C21H44	000629-94-7	86
4	Octacosane	394	C28H58	000630-02-4	86
5	Sulfurous acid, 2-propyl tetra...	320	C17H36O3S	1000309-12-5	86



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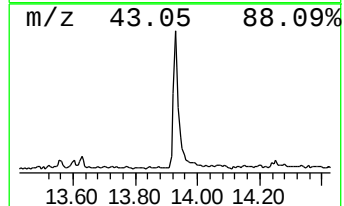
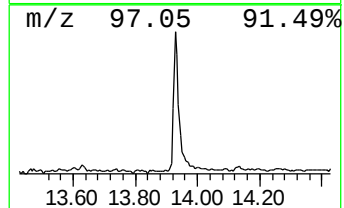
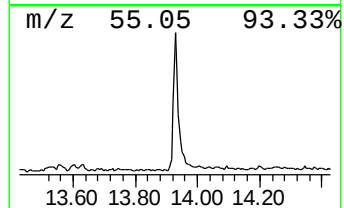
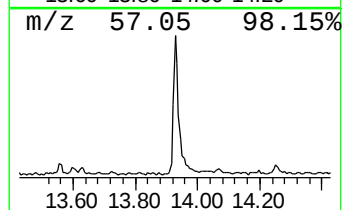
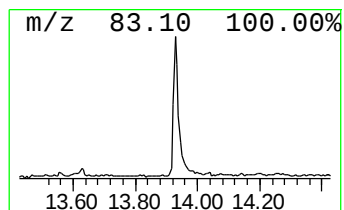
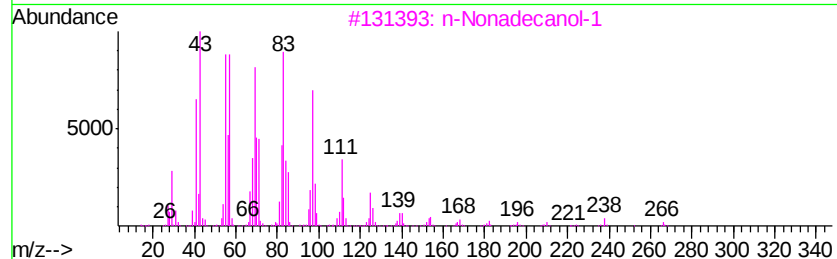
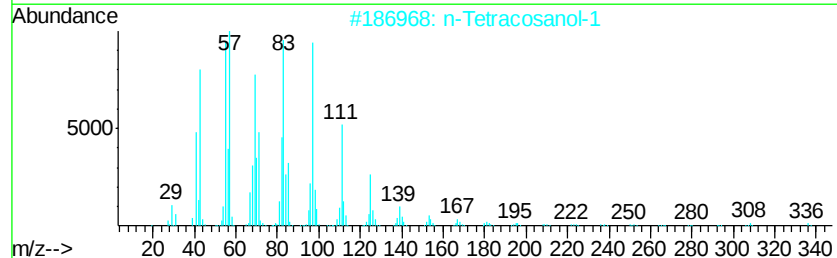
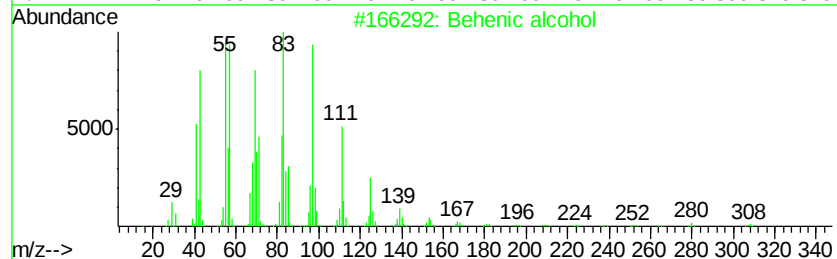
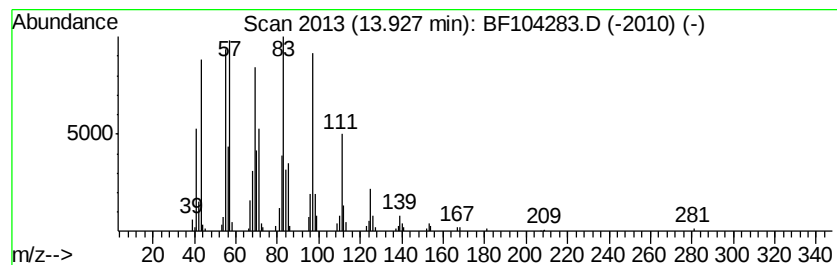
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	7.22 ng	335769	Chrysene-d12	14.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	95
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4		1-Heptacosanol	396	C27H56O	002004-39-9	95
5		1-Heneicosanol	312	C21H44O	015594-90-8	95



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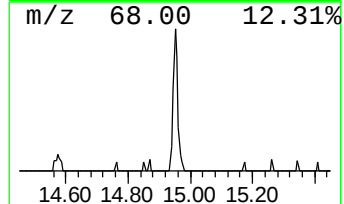
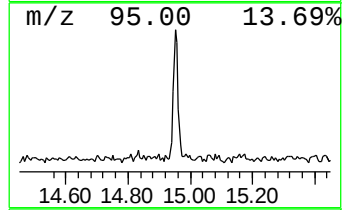
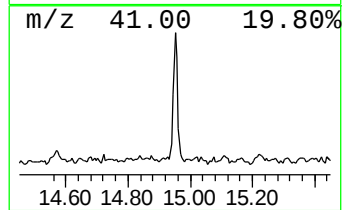
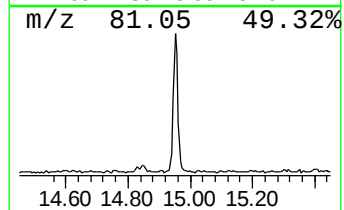
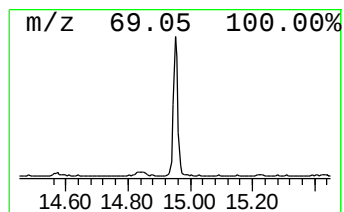
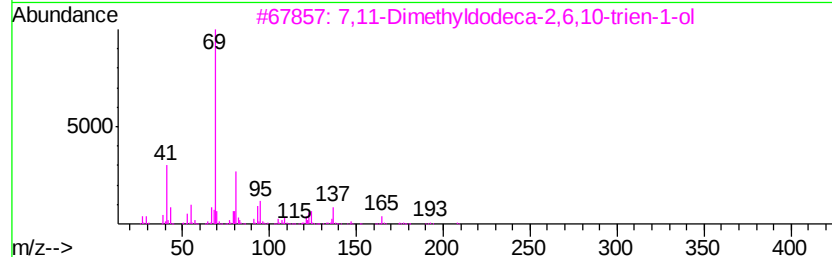
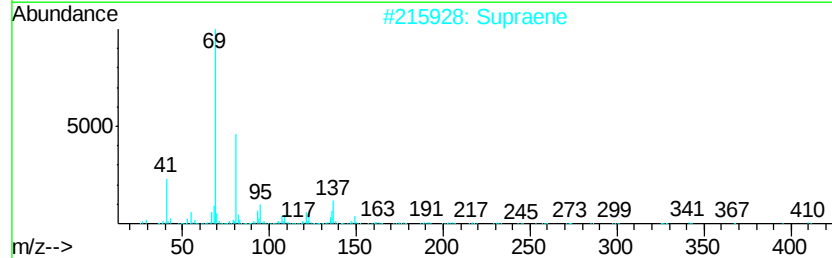
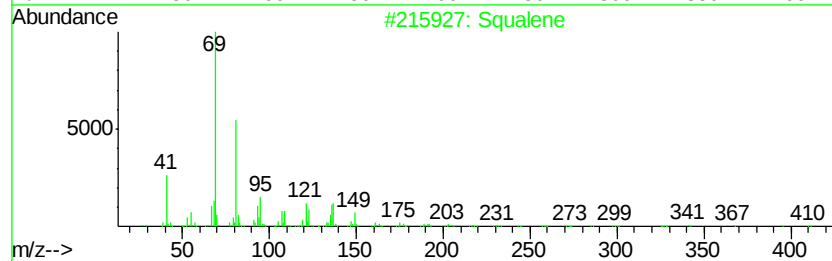
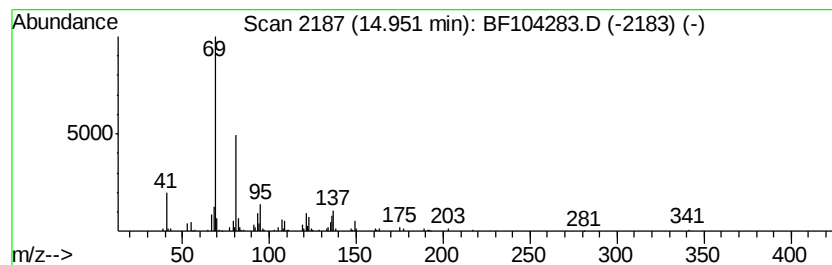
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	4.73 ng	154996	Perylene-d12	15.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040518\
Data File : BF104283.D
Acq On : 5 Apr 2018 21:27
Operator : JU/SJ
Sample : J2237-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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...	2.28	6.0	ng	164983	1	6.95	547152	20.0
2-Pentanone, 4-hy...	5.19	2.6	ng	70821	1	6.95	547152	20.0
unknown6.72	6.72	109.2	ng	2987030	1	6.95	547152	20.0
Nonadecane	10.86	3.3	ng	163592	4	11.48	1000490	20.0
Behenic alcohol	13.93	7.2	ng	335769	5	14.13	929860	20.0
Squalene	14.95	4.7	ng	154996	6	15.66	655650	20.0