

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050817\
 Data File : BF094992.D
 Acq On : 8 May 2017 21:41
 Operator : SJ/MA
 Sample : I3011-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BP-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-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	5.031	521	526	541	rBV	267492	563668	16.52%	2.139%
2	5.660	628	633	657	rBV	1770766	2602706	76.26%	9.875%
3	7.260	899	905	919	rBV	1812684	2709487	79.39%	10.280%
4	7.378	919	925	935	rVB	2234491	2933877	85.96%	11.131%
5	7.713	978	982	994	rBV	469096	550789	16.14%	2.090%
6	7.954	1018	1023	1043	rVB	1997991	2388717	69.99%	9.063%
7	8.613	1130	1135	1168	rBV	1313716	1880517	55.10%	7.135%
8	9.736	1321	1326	1339	rBV	553108	775538	22.72%	2.942%
9	11.513	1622	1628	1646	rBV	2693097	3412910	100.00%	12.949%
10	12.201	1740	1745	1752	rBV	230847	313017	9.17%	1.188%
11	12.560	1802	1806	1816	rBV2	540945	793722	23.26%	3.011%
12	13.407	1946	1950	1956	rBV	42013	49322	1.45%	0.187%
13	13.859	2021	2027	2041	rBV	1280644	1834402	53.75%	6.960%
14	14.177	2077	2081	2084	rBV	33779	40641	1.19%	0.154%
15	14.965	2210	2215	2227	rBV	575197	776204	22.74%	2.945%
16	15.930	2374	2379	2389	rBV2	134499	189934	5.57%	0.721%
17	17.018	2560	2564	2571	rBV2	51106	77247	2.26%	0.293%
18	17.295	2605	2611	2614	rBV	2282025	2670685	78.25%	10.133%
19	18.577	2825	2829	2834	rBV7	16028	38953	1.14%	0.148%
20	18.630	2834	2838	2846	rVV	460158	583248	17.09%	2.213%
21	18.694	2846	2849	2854	rVB	90638	94444	2.77%	0.358%
22	19.659	3009	3013	3017	rBV4	27767	44468	1.30%	0.169%
23	20.047	3075	3079	3084	rBV	57735	72863	2.13%	0.276%
24	20.294	3117	3121	3135	rVB	413129	554621	16.25%	2.104%
25	20.771	3198	3202	3206	rBV	46831	57447	1.68%	0.218%
26	20.883	3212	3221	3228	rBV	18817	53097	1.56%	0.201%
27	21.683	3352	3357	3363	rBV7	23798	49957	1.46%	0.190%
28	22.488	3489	3494	3503	rVB9	26479	65418	1.92%	0.248%
29	22.741	3529	3537	3555	rVB9	25297	119479	3.50%	0.453%
30	23.724	3694	3704	3706	rBV6	26544	59178	1.73%	0.225%

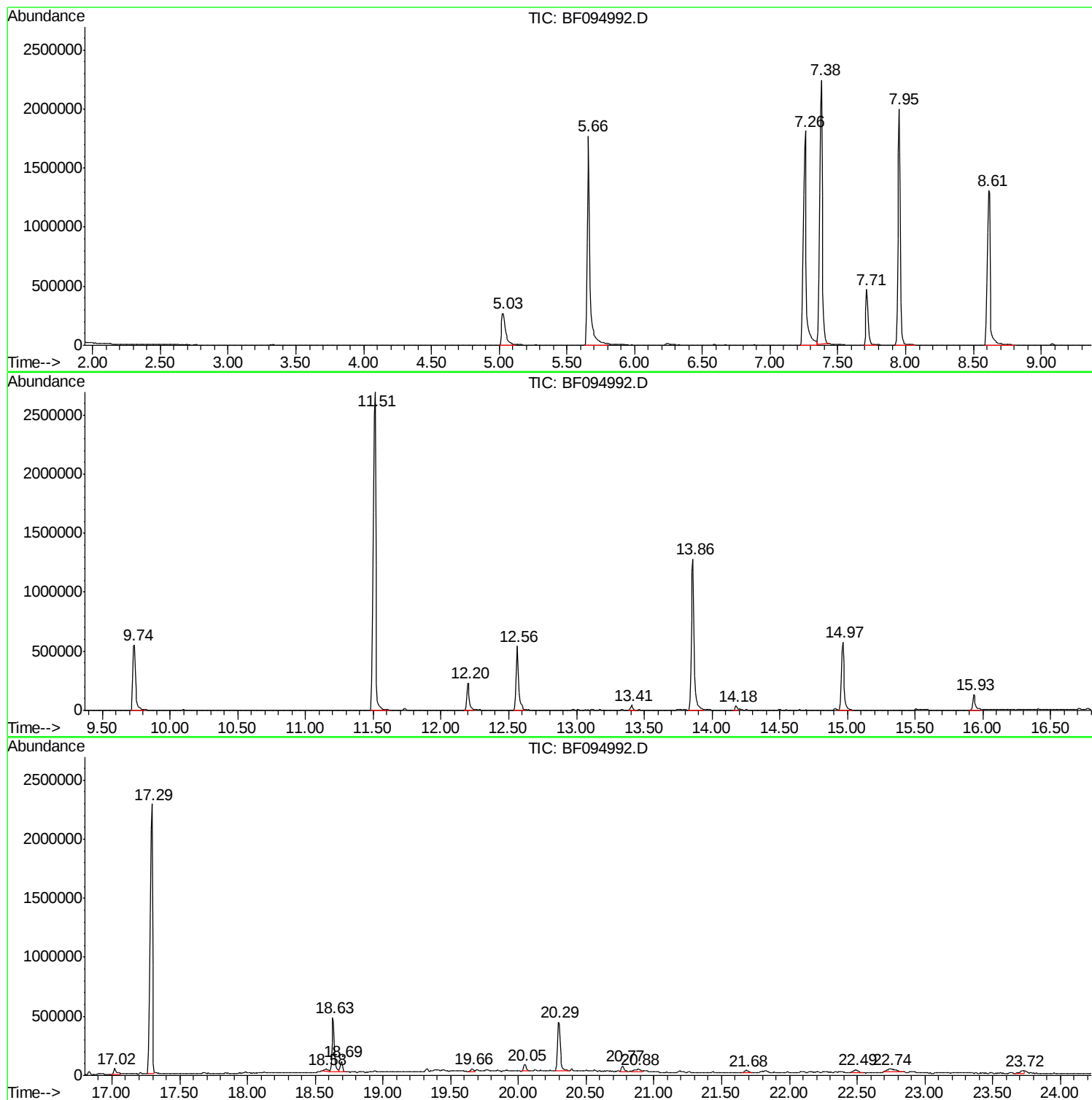
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
BP-1

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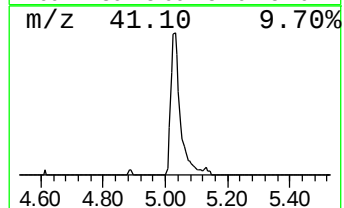
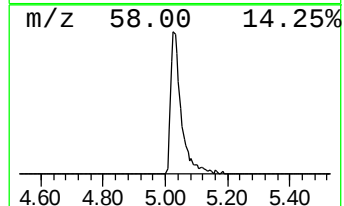
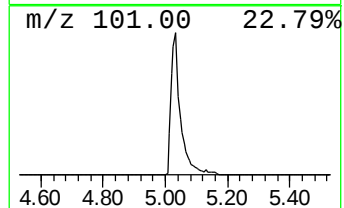
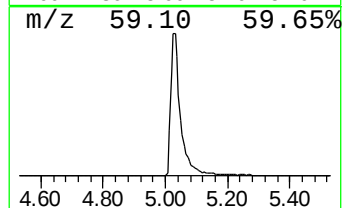
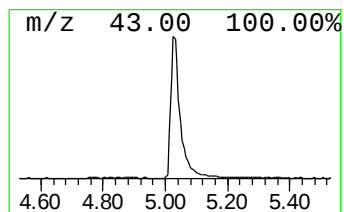
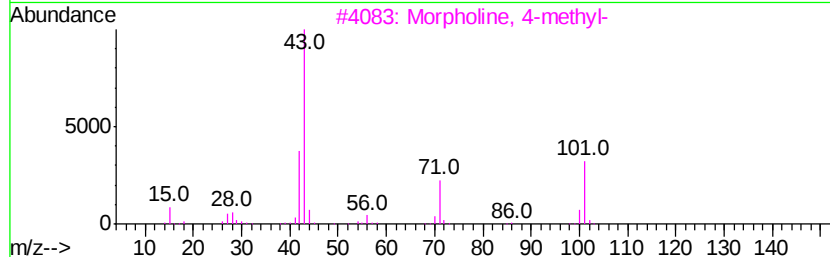
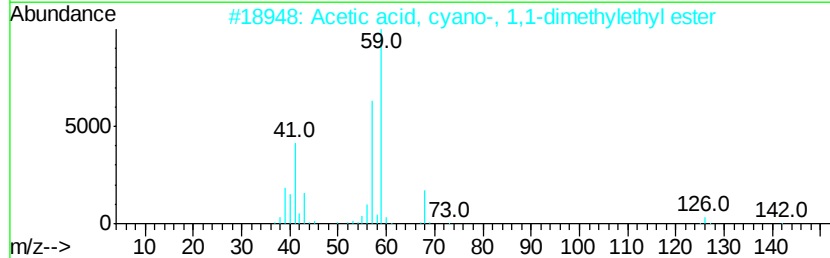
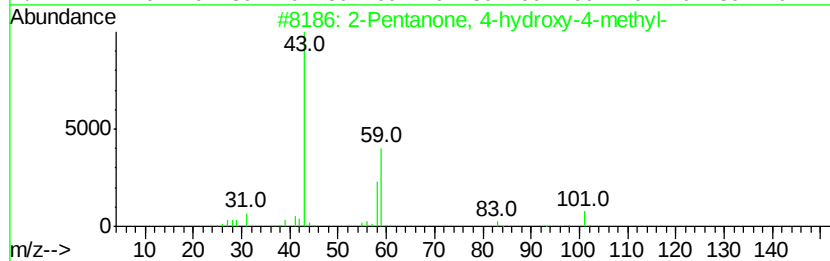
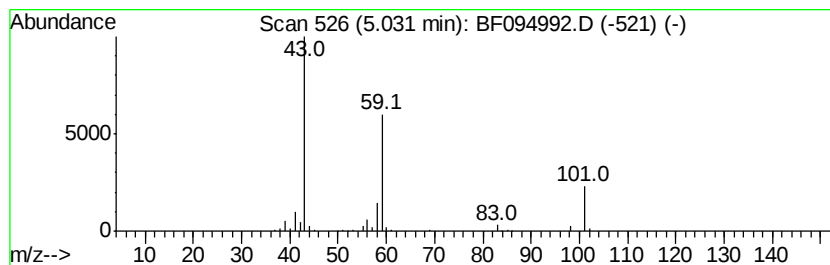
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.03	20.47 ng	563668	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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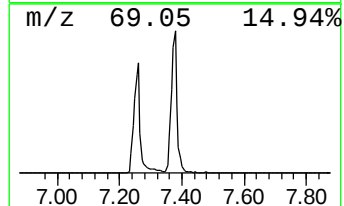
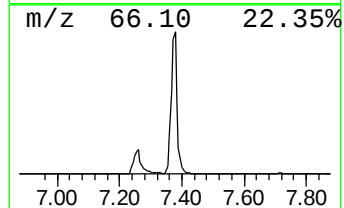
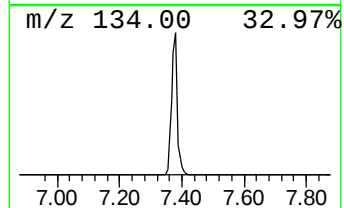
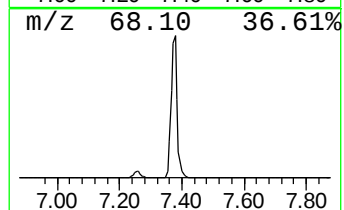
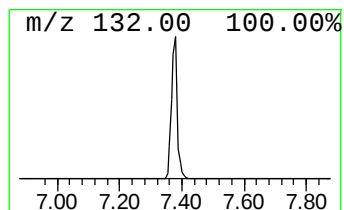
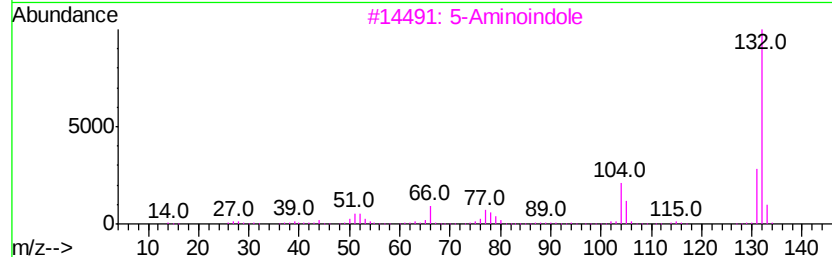
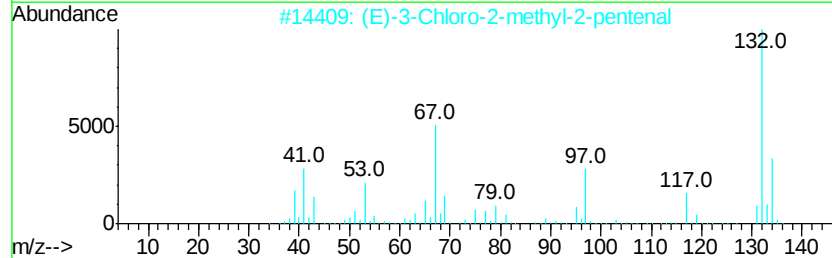
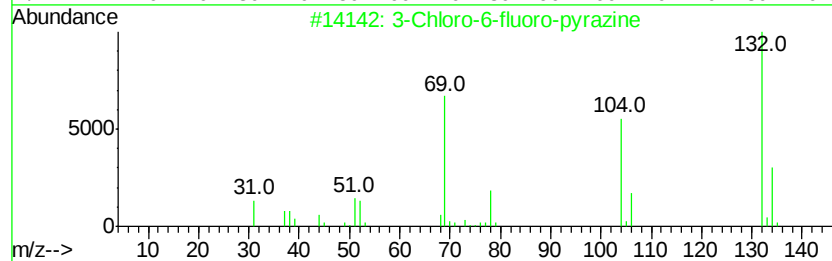
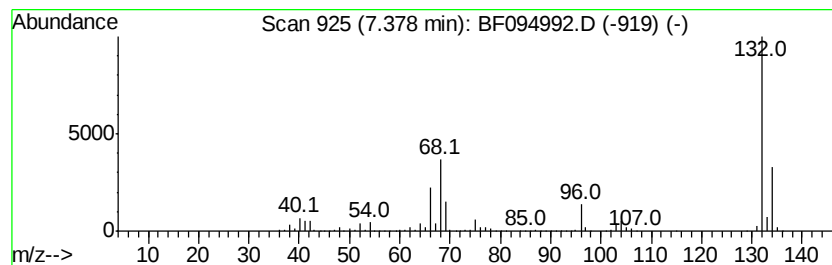
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	106.53 ng	2933880	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		Xenon	132	Xe	007440-63-3	9



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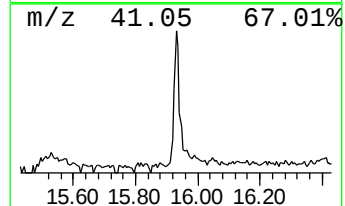
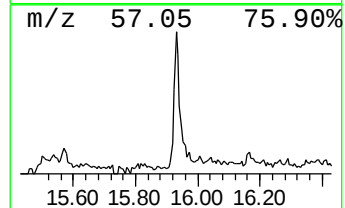
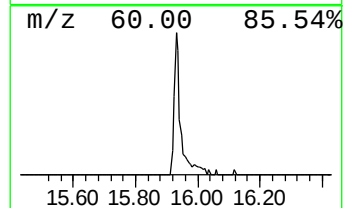
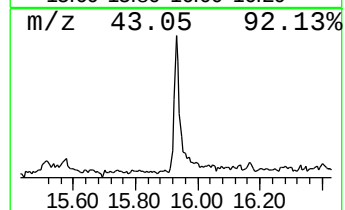
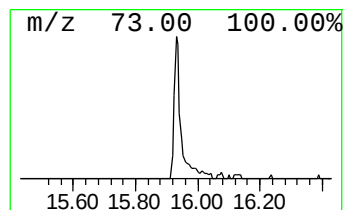
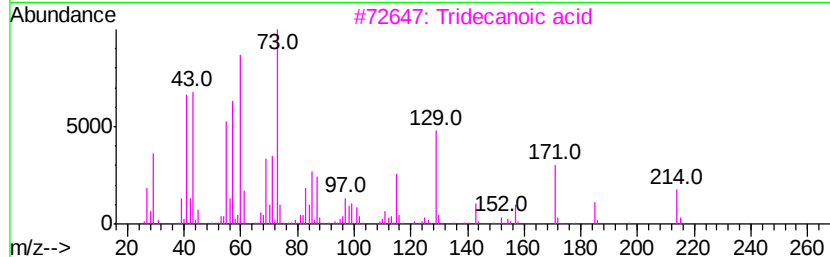
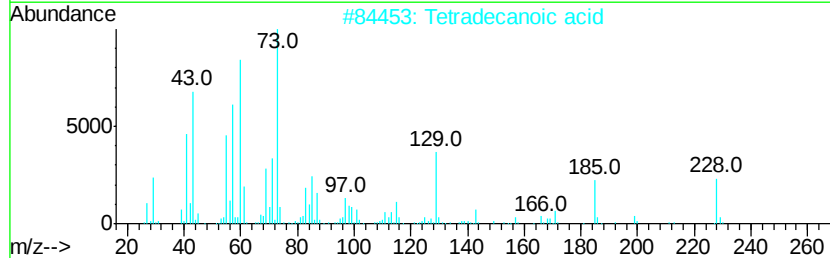
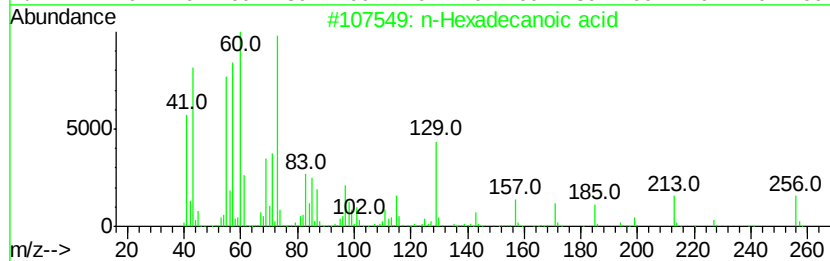
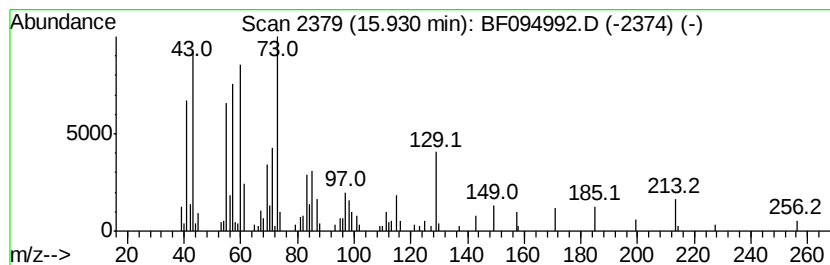
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	4.89 ng	189934	Phenanthrene-d10	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3		Tridecanoic acid	214	C13H26O2	000638-53-9	76
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	20



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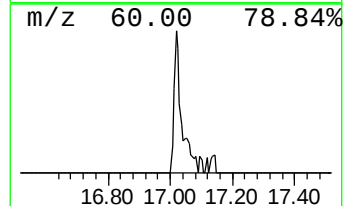
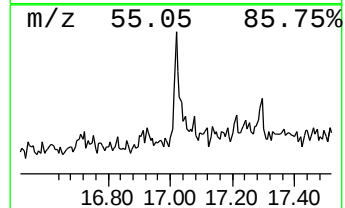
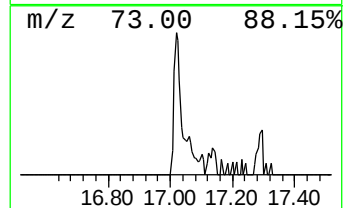
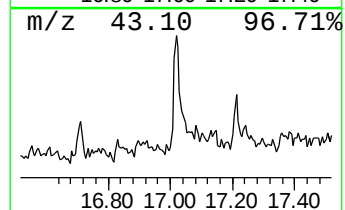
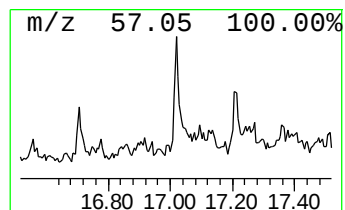
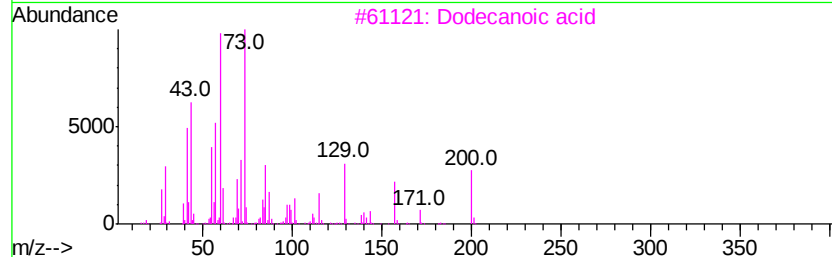
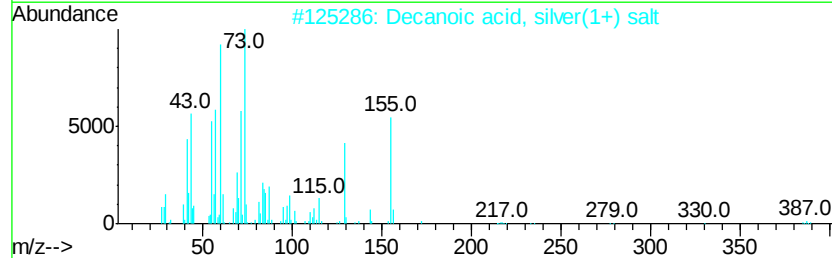
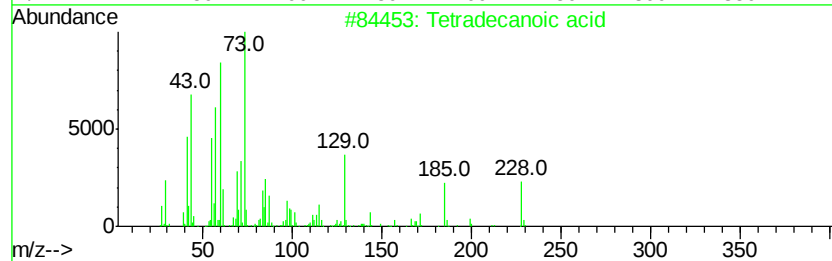
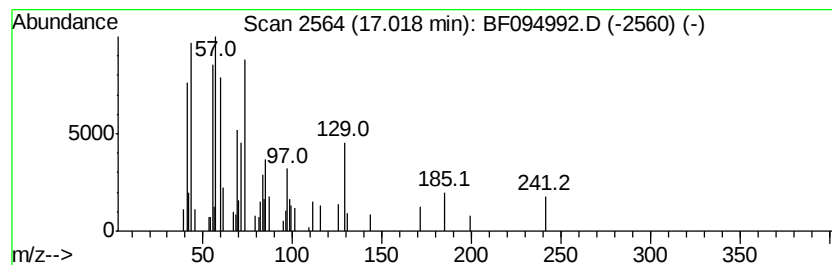
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.02	2.65 ng	77247	Chrysene-d12	18.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
2		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58
3		Dodecanoic acid	200	C12H24O2	000143-07-7	47
4		n-Decanoic acid	172	C10H20O2	000334-48-5	47
5		Octacosyl acetate	452	C30H60O2	018206-97-8	11



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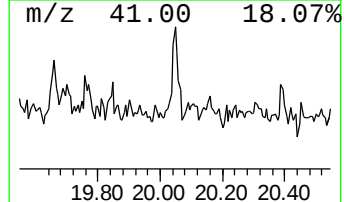
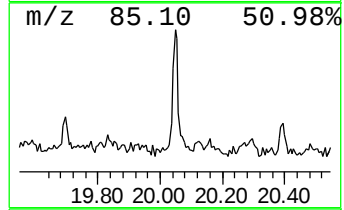
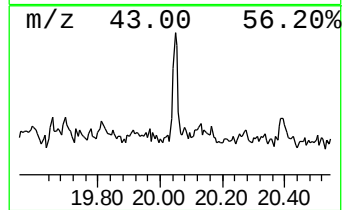
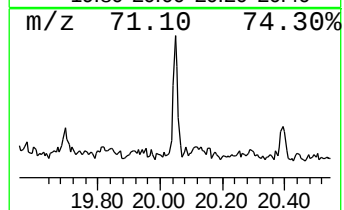
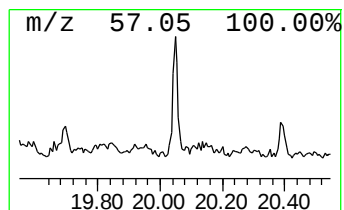
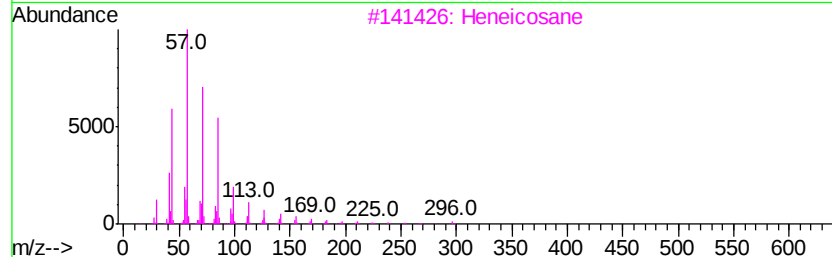
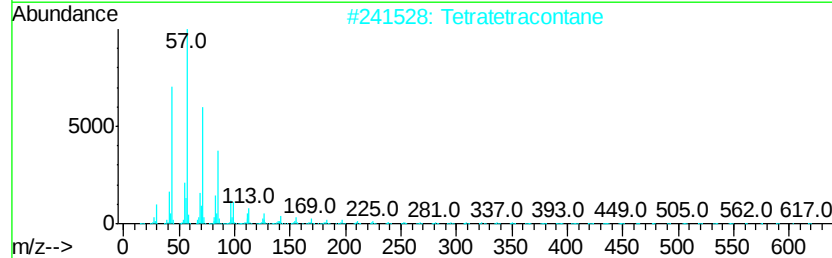
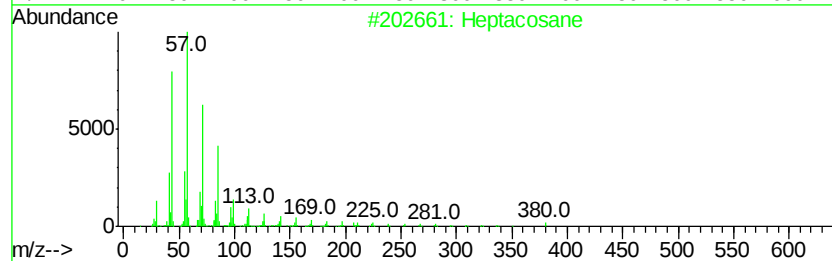
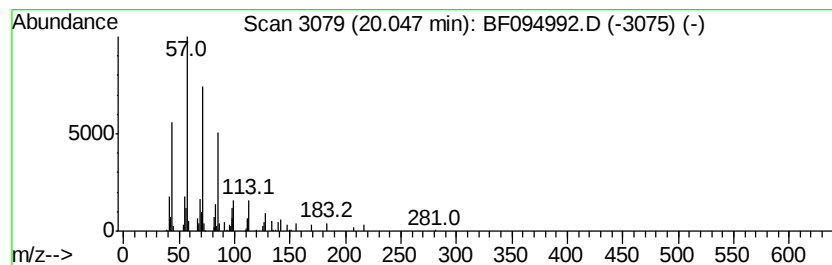
Instrument :
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Peak Number 6 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
20.05	2.63 ng	72863	Perylene-d12		20.30
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octadecane	254	C18H38	000593-45-3	91
5	Heptadecane	240	C17H36	000629-78-7	90



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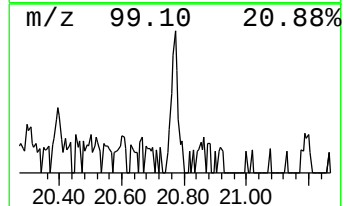
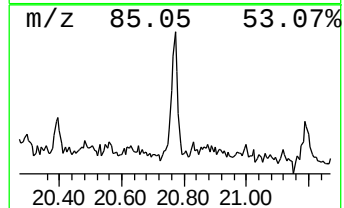
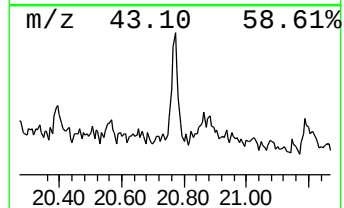
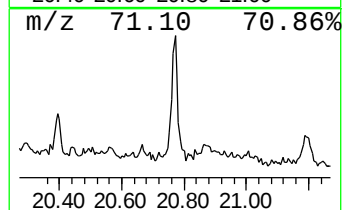
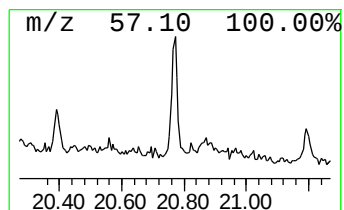
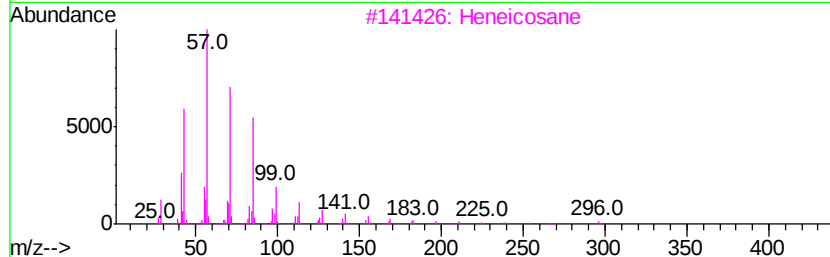
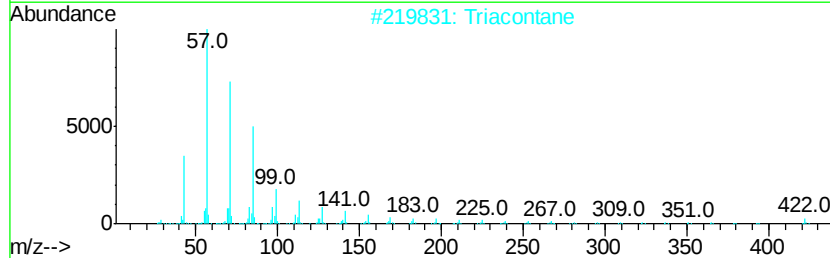
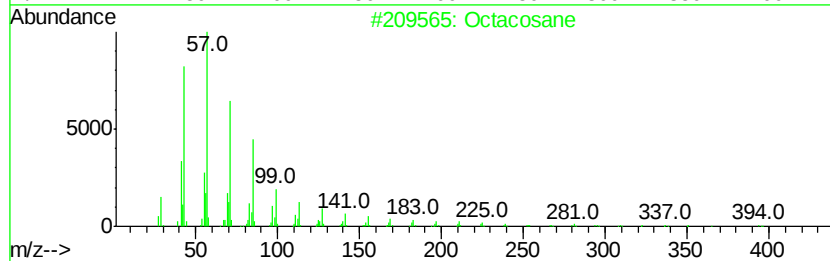
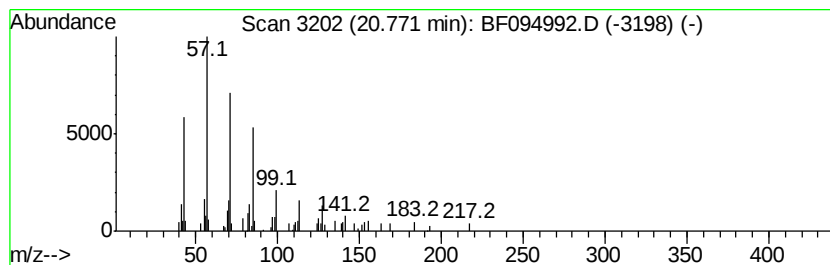
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.77	2.07 ng	57447	Perylene-d12	20.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	87
2	triacontane		422	C30H62	000638-68-6	86
3	Heneicosane		296	C21H44	000629-94-7	83
4	Hexacosane		366	C26H54	000630-01-3	83
5	Heptadecane		240	C17H36	000629-78-7	80



Data Path : Z:\HPCHEM1\BNA F\DATA\BF050817\
Data File : BF094992.D
Acq On : 8 May 2017 21:41
Operator : SJ/MA
Sample : I3011-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
BP-1

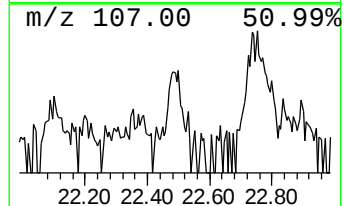
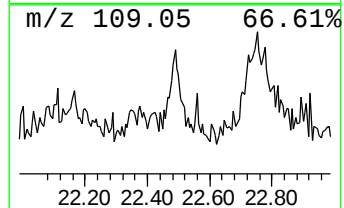
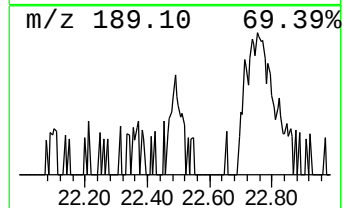
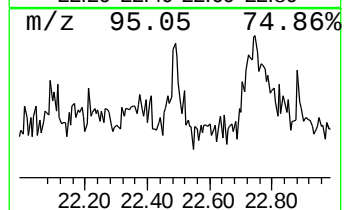
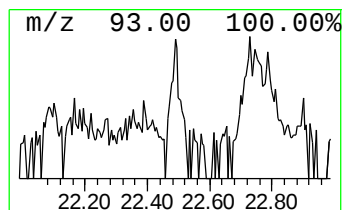
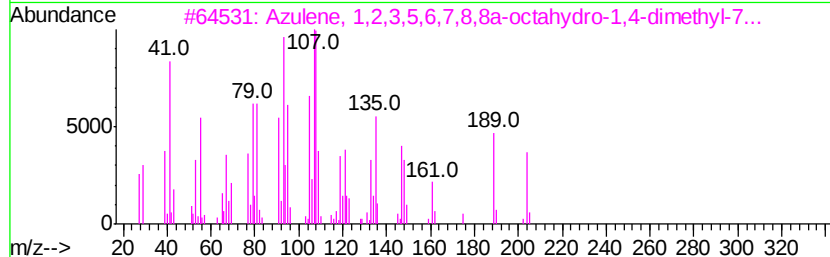
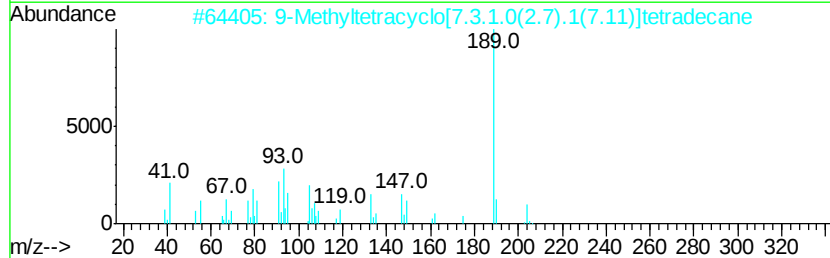
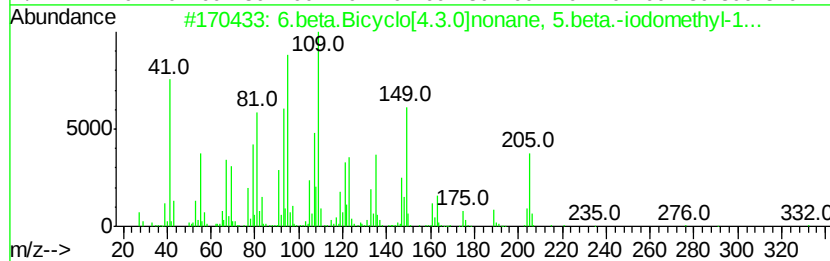
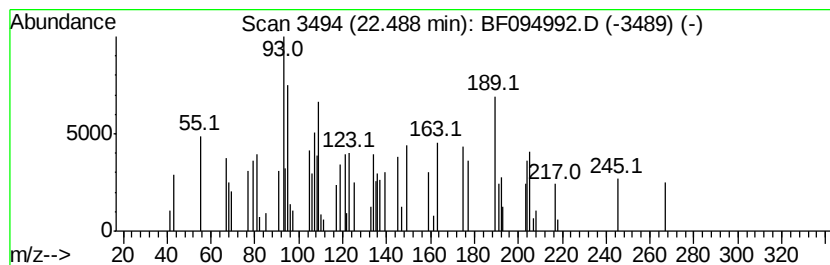
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown22.49 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.49	2.36 ng	65418	Perylene-d12	20.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6	beta	Bicyclo[4.3.0]nonane, 5.b...	332	C15H25I	1000195-85-9	27
2	9	Methyl	tetracyclo[7.3.1.0(2.7)...	204	C15H24	1000215-30-5	20
3	Azulene, 1,2,3,5,6,7,8,8a-octahv...	204	C15H24	003691-11-0	18		
4	1,8-Nonadiene, 2,7-dimethyl-5-(1...	192	C14H24	068702-20-5	14		
5	[1,2,4]Triazolo[1,5-a]pyrimidine...	208	C9H12N4S	1000304-66-8	14		



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Sample : I3011-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
BP-1

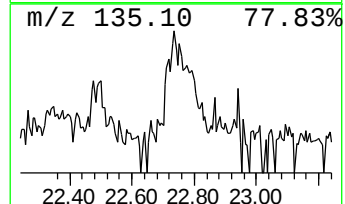
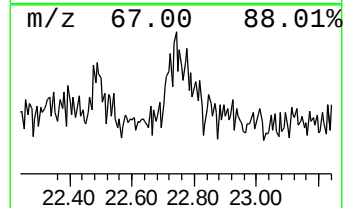
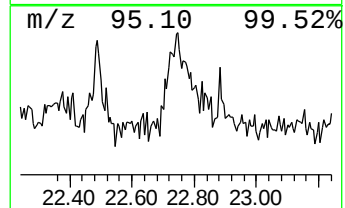
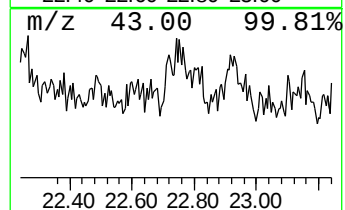
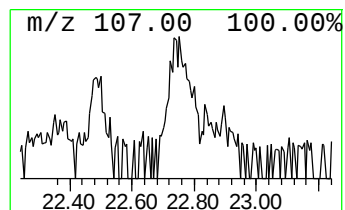
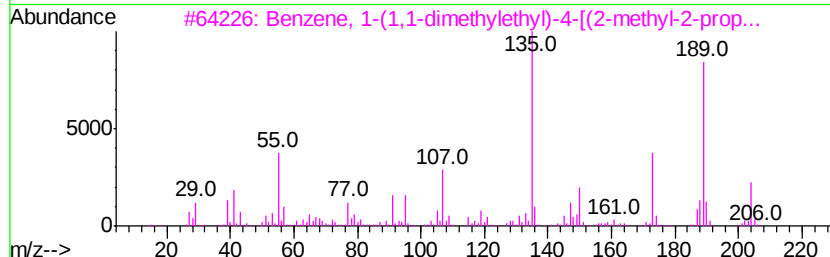
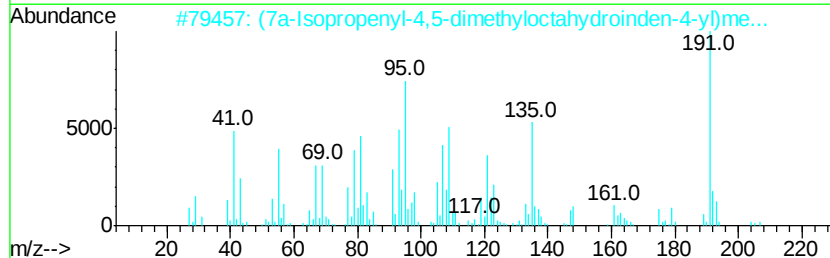
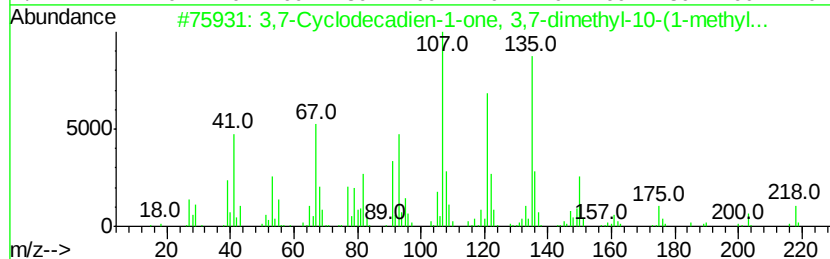
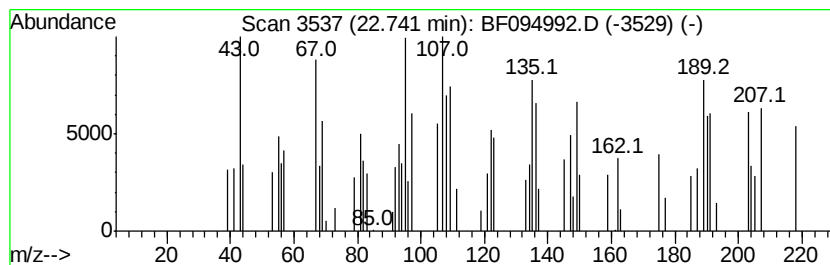
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown22.74 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.74	4.31 ng	119479	Perylene-d12	20.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,7-Cyclodecadien-1-one, 3,7-dim...	218	C15H22O	006902-91-6	38		
2	(7a-Isopropenyl-4,5-dimethylocta...	222	C15H26O	1000187-02-9	38		
3	Benzene, 1-(1,1-dimethylethyl)-4...	204	C14H20O	054932-87-5	35		
4	9,9'-Biphenanthrene, octacosahydro-	382	C28H46	055334-18-4	27		
5	2-Methylisoborneol	168	C11H20O	002371-42-8	22		



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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampled :
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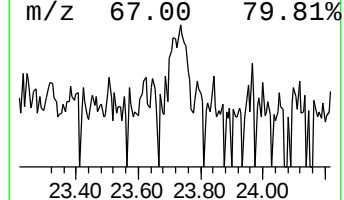
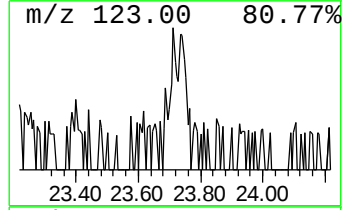
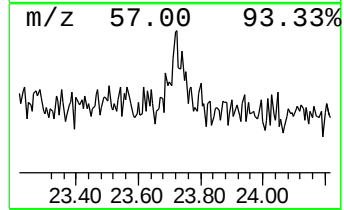
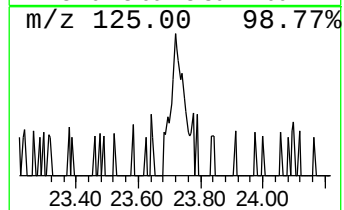
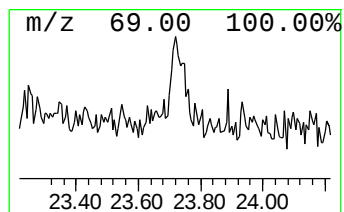
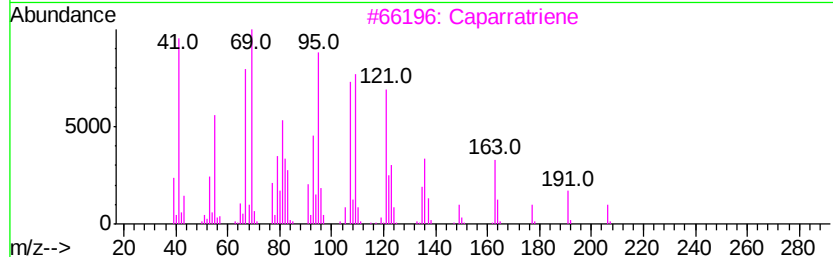
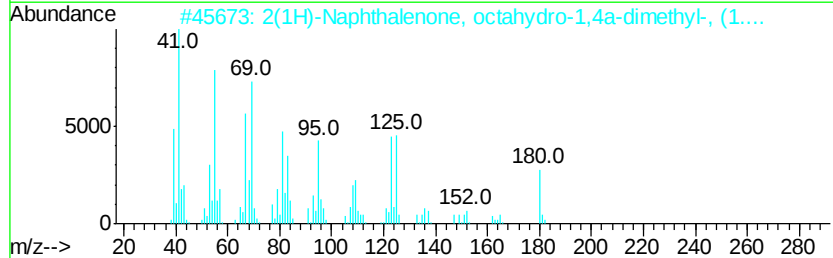
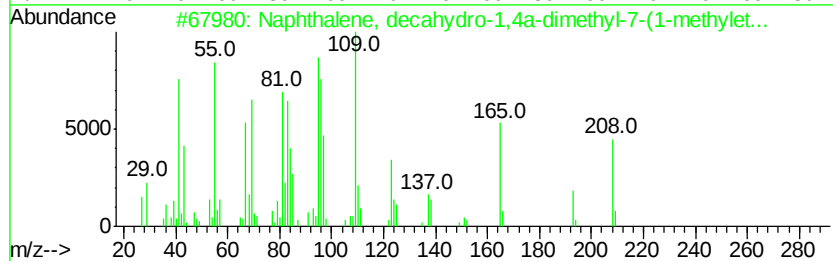
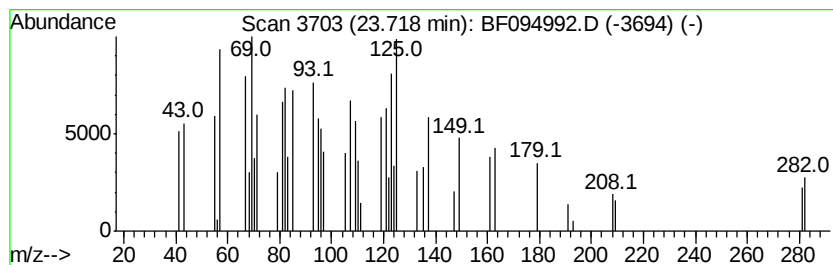
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Naphthalene, decahydro-1,4a... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.72	2.13 ng	59178	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, decahydro-1,4a-dime...	208	C15H28	030824-81-8	50
2		2(1H)-Naphthalenone, octahydro-1...	180	C12H20O	022738-31-4	25
3		Caparratriene	206	C15H26	1000374-08-7	22
4		Tridecanal	198	C13H26O	010486-19-8	18
5		2H-Pyran, 2-(7-heptadecynyloxy)t...	336	C22H40O2	056599-50-9	15



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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.03	20.5	ng	563668	1	7.71	550789	20.0
unknown7.38	7.38	106.5	ng	2933880	1	7.71	550789	20.0
n-Hexadecanoic acid	15.93	4.9	ng	189934	4	14.97	776204	20.0
Tetradecanoic acid	17.02	2.6	ng	77247	5	18.63	583248	20.0
Heptacosane	20.05	2.6	ng	72863	6	20.30	554621	20.0
Octacosane	20.77	2.1	ng	57447	6	20.30	554621	20.0
unknown22.49	22.49	2.4	ng	65418	6	20.30	554621	20.0
unknown22.74	22.74	4.3	ng	119479	6	20.30	554621	20.0
Naphthalene, deca...	23.72	2.1	ng	59178	6	20.30	554621	20.0