

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050217\
 Data File : BF094820.D
 Acq On : 3 May 2017 6:44
 Operator : SJ/MA
 Sample : PB98658BL
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB98658BL

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-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	4.131	368	373	387	rBV	57388	114370	3.92%	0.514%
2	5.048	523	529	544	rBV	458467	908325	31.11%	4.080%
3	5.689	633	638	661	rBV	1778333	2475658	84.80%	11.120%
4	6.248	729	733	743	rBV	27142	42766	1.46%	0.192%
5	7.278	902	908	923	rBV	1734173	2329966	79.81%	10.466%
6	7.395	923	928	943	rVB	2073888	2586379	88.59%	11.618%
7	7.730	981	985	993	rBV	497452	545863	18.70%	2.452%
8	7.972	1020	1026	1038	rBV	1753637	2005547	68.69%	9.009%
9	8.630	1131	1138	1155	rBV	1148853	1511986	51.79%	6.792%
10	9.748	1324	1328	1345	rVB	607603	703731	24.10%	3.161%
11	11.524	1624	1630	1634	rBV	2418544	2919497	100.00%	13.114%
12	12.577	1804	1809	1824	rBV2	562231	743358	25.46%	3.339%
13	13.871	2024	2029	2049	rBV	980123	1367010	46.82%	6.140%
14	14.977	2212	2217	2228	rBV	518065	650342	22.28%	2.921%
15	17.306	2608	2613	2617	rBV	1947967	2211627	75.75%	9.934%
16	18.642	2836	2840	2850	rBV	443354	499951	17.12%	2.246%
17	20.306	3119	3123	3130	rBV2	382657	441022	15.11%	1.981%
18	20.418	3138	3142	3148	rVB2	33443	41205	1.41%	0.185%
19	20.794	3200	3206	3211	rBV2	40935	60436	2.07%	0.271%
20	21.224	3275	3279	3284	rVB2	34872	53180	1.82%	0.239%
21	21.718	3359	3363	3370	rVB3	24560	50188	1.72%	0.225%

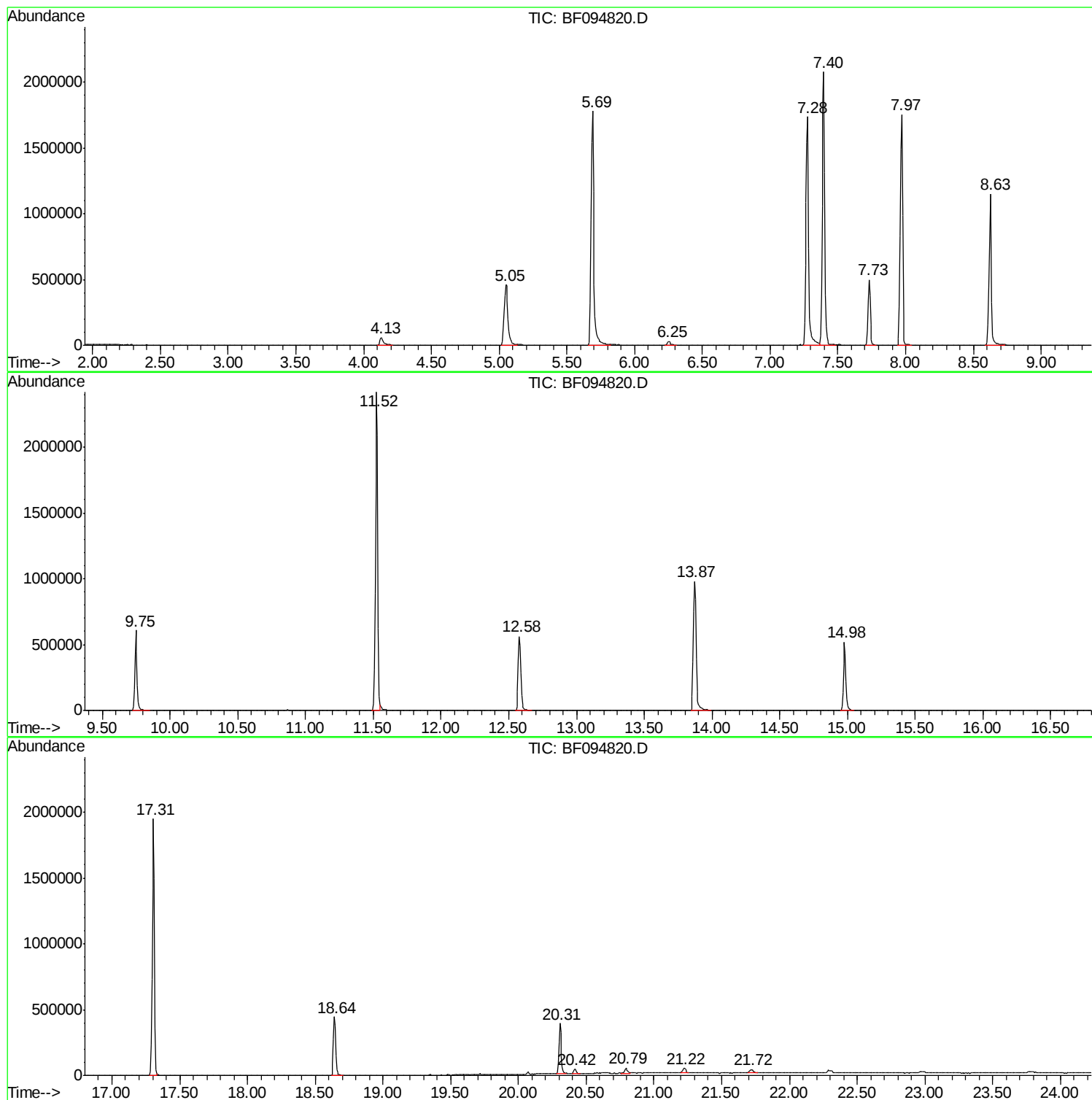
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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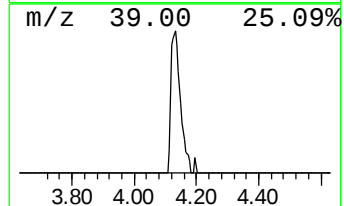
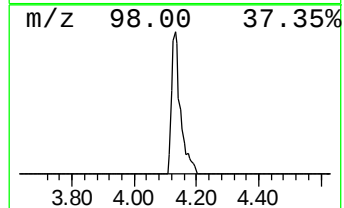
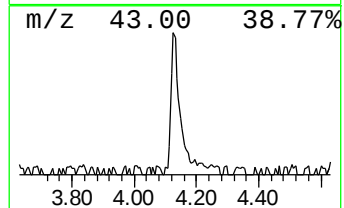
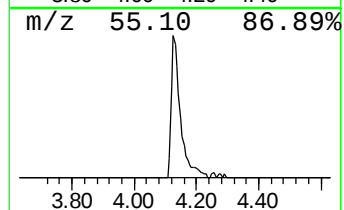
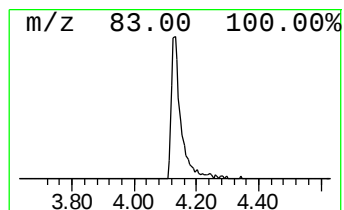
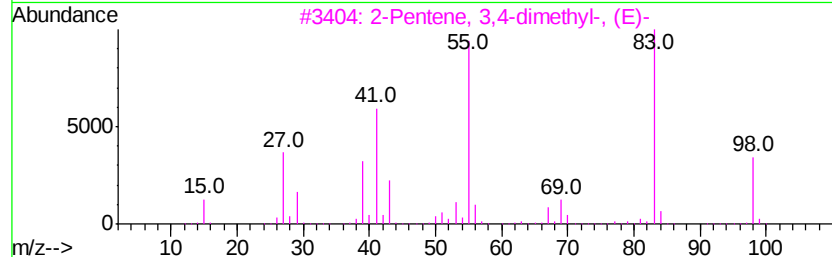
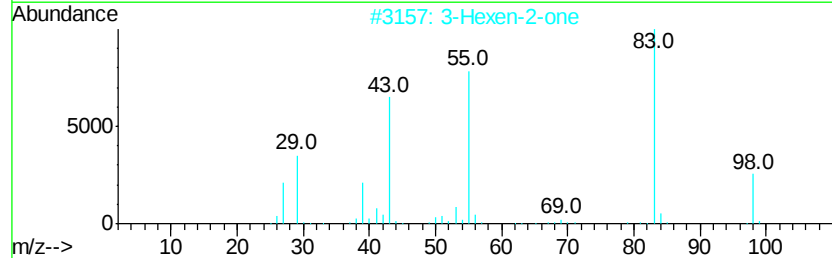
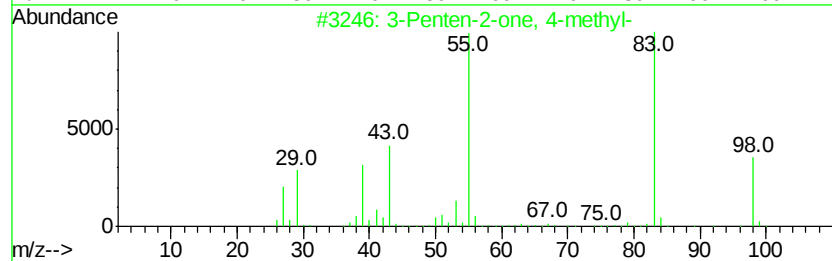
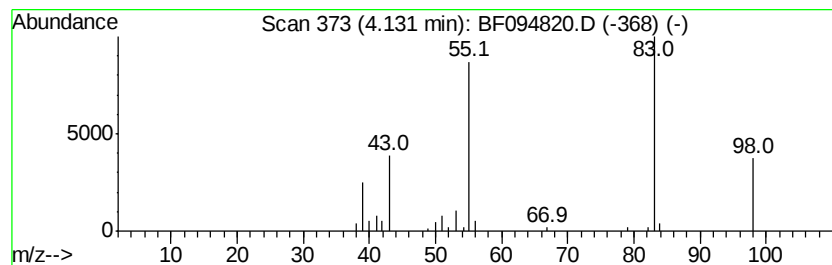
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.13	4.19 ng	114370	1,4-Dichlorobenzene-d4	7.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	86
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	72
4			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	64
5			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	64



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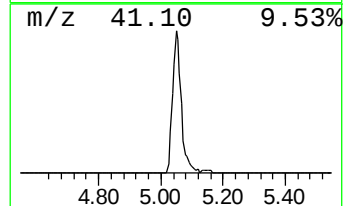
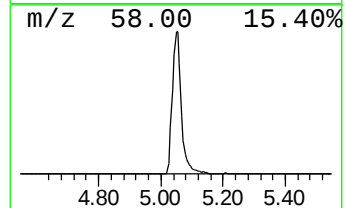
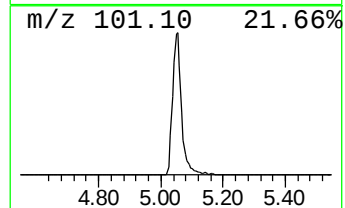
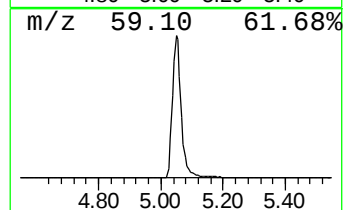
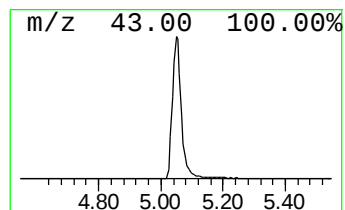
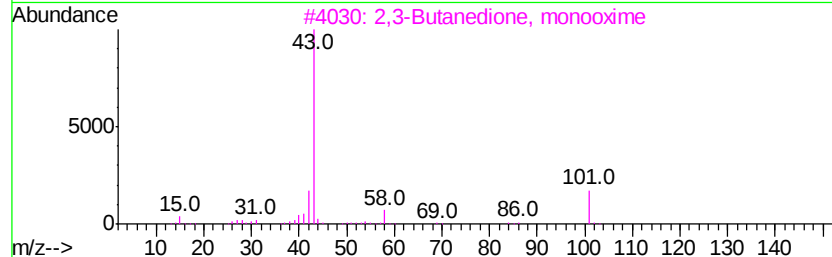
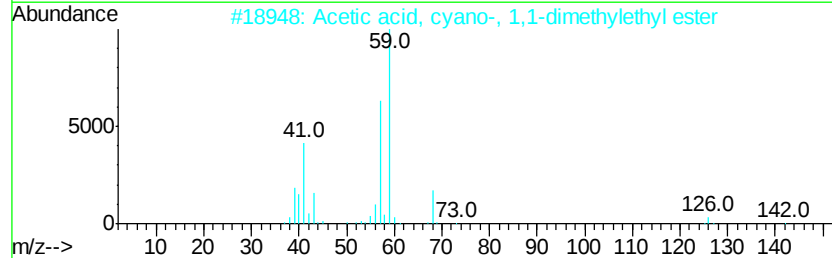
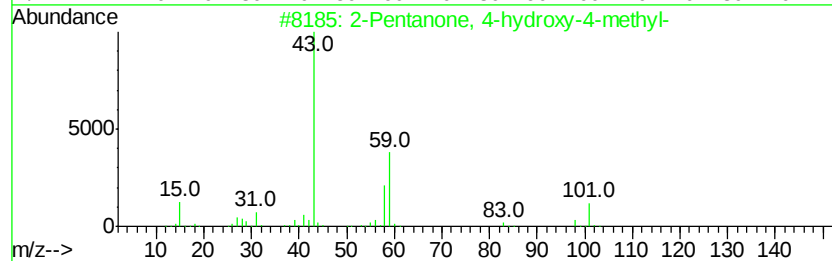
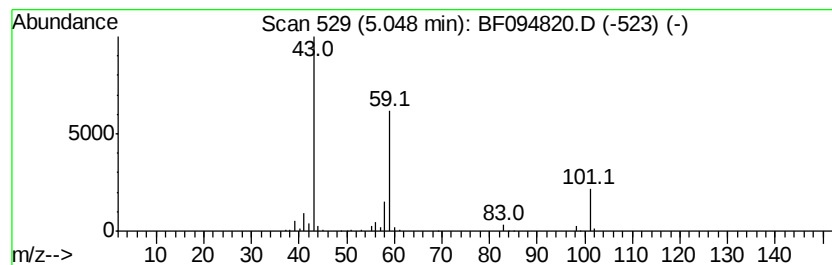
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	33.28 ng	908325	1,4-Dichlorobenzene-d4	7.73

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, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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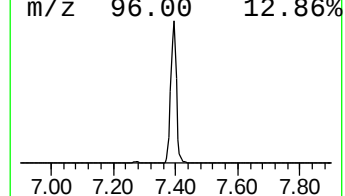
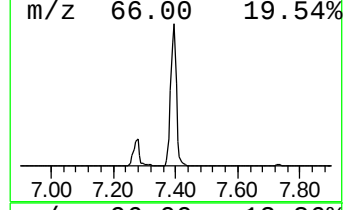
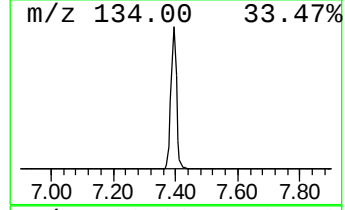
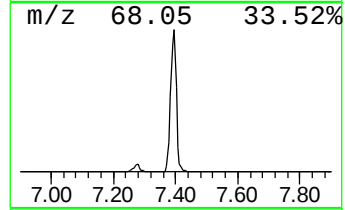
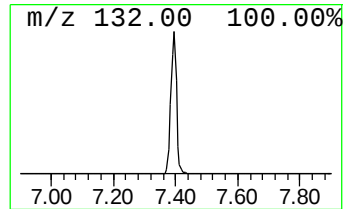
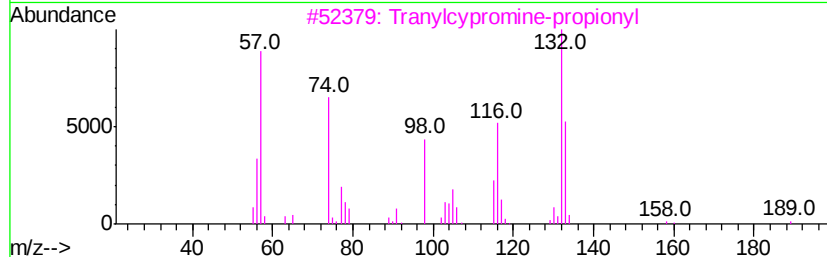
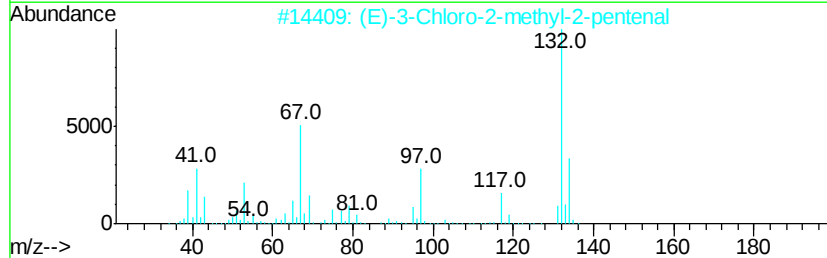
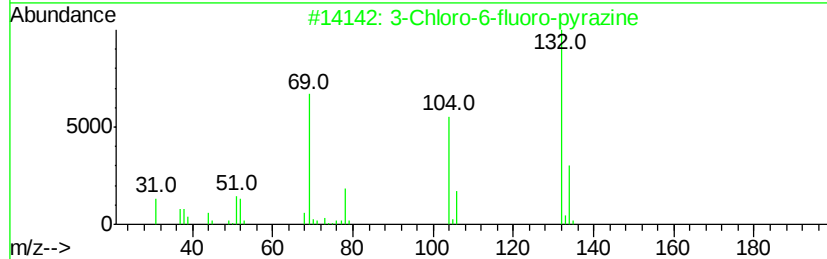
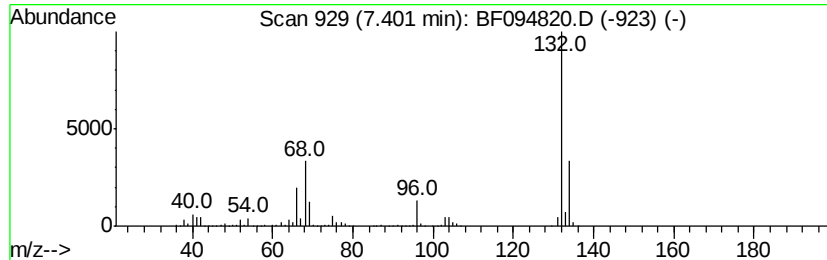
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TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.40	94.76 ng	2586380	1,4-Dichlorobenzene-d4	7.73

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	25
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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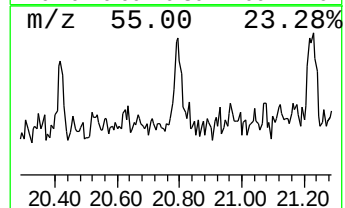
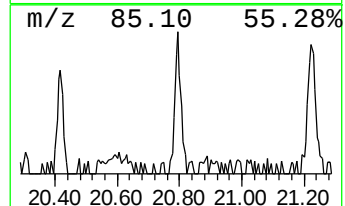
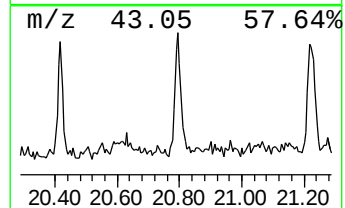
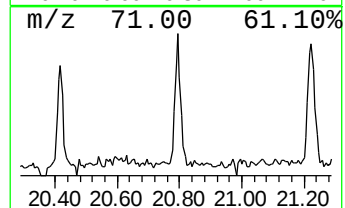
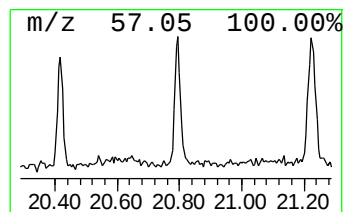
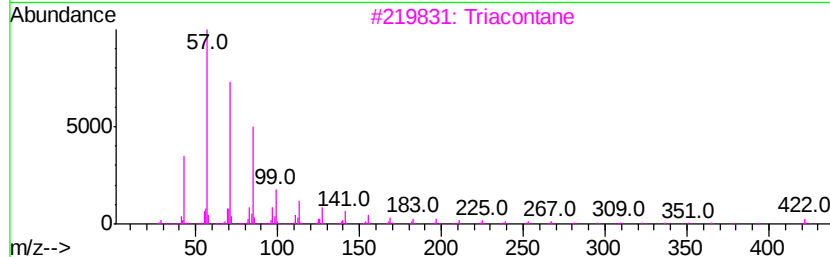
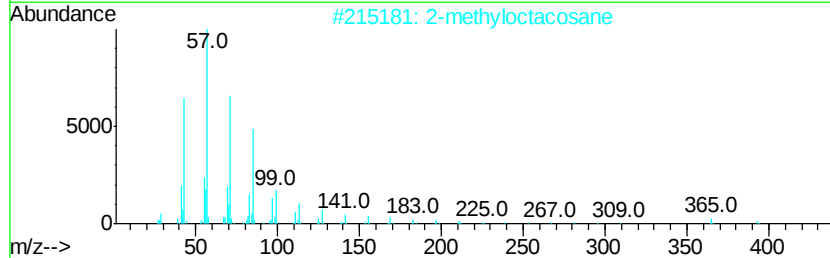
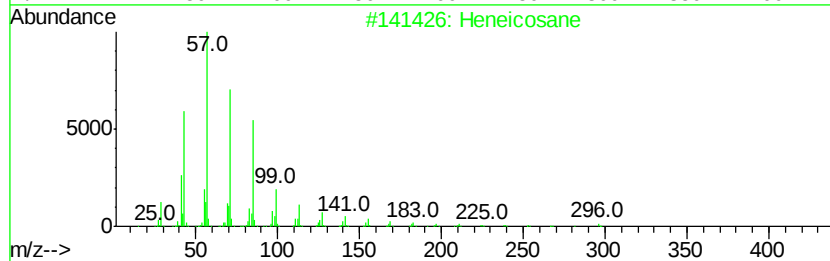
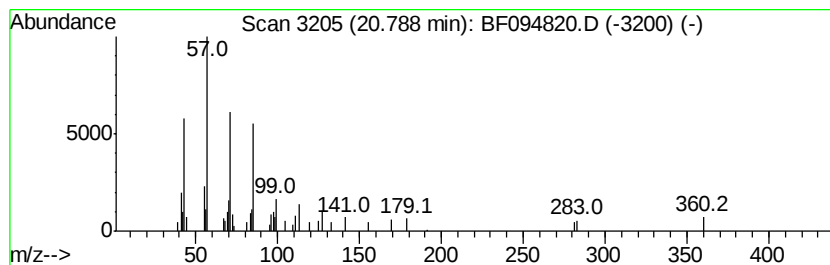
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.79	2.74 ng	60436	Perylene-d12	20.31

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	87
2	2-methyloctacosane		408	C29H60	1000376-72-8	87
3	triacontane		422	C30H62	000638-68-6	86
4	Eicosane		282	C20H42	000112-95-8	86
5	Tetracosane		338	C24H50	000646-31-1	86



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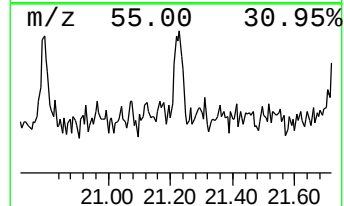
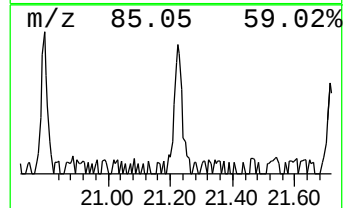
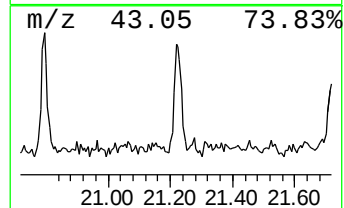
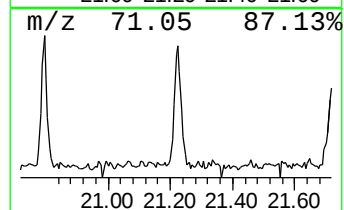
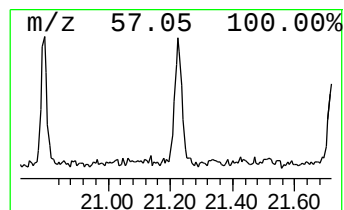
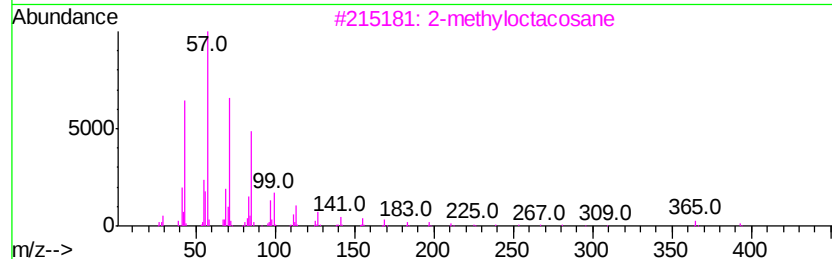
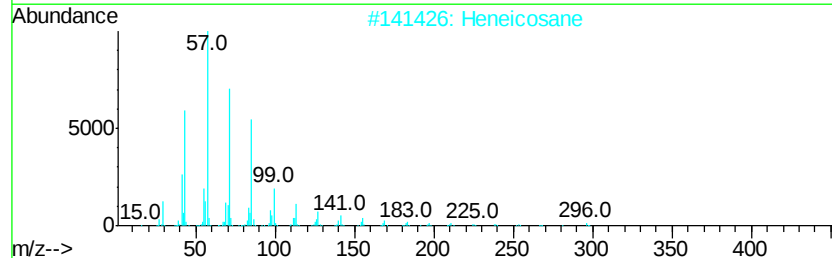
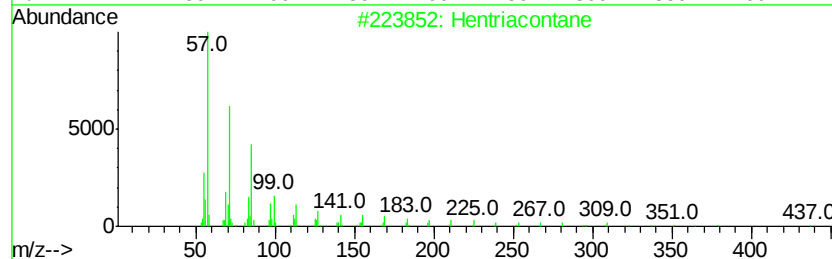
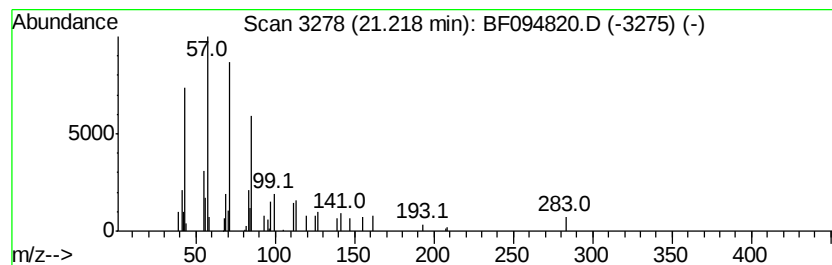
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.22	2.41 ng	53180	Perylene-d12	20.31

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	91
2	Heneicosane		296	C21H44	000629-94-7	90
3	2-methyloctacosane		408	C29H60	1000376-72-8	90
4	Octacosane		394	C28H58	000630-02-4	87
5	Pentacosane		352	C25H52	000629-99-2	87



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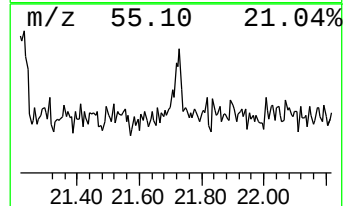
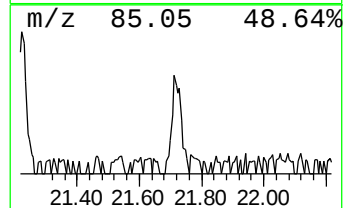
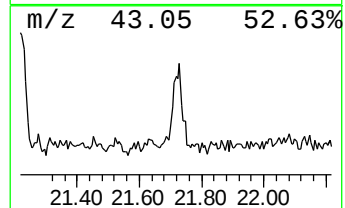
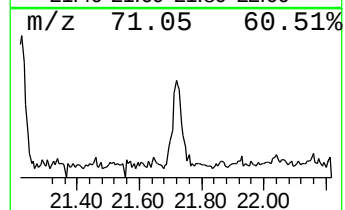
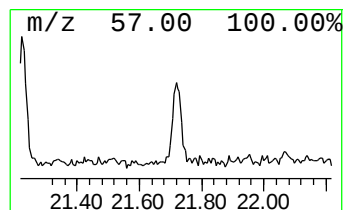
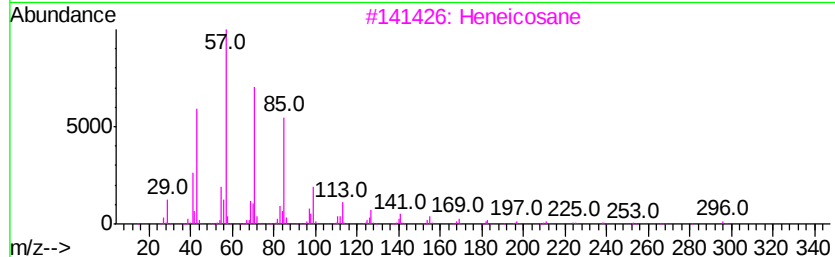
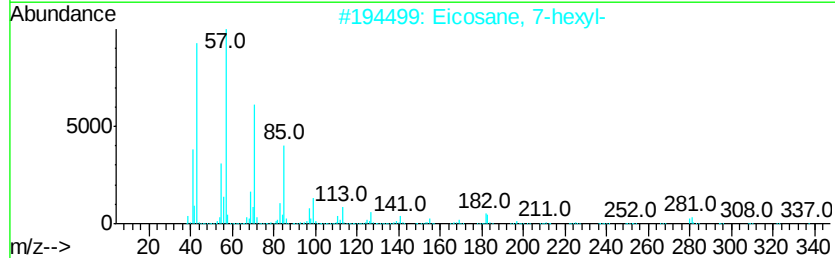
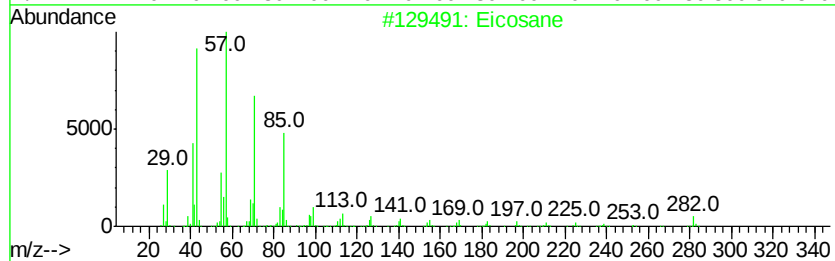
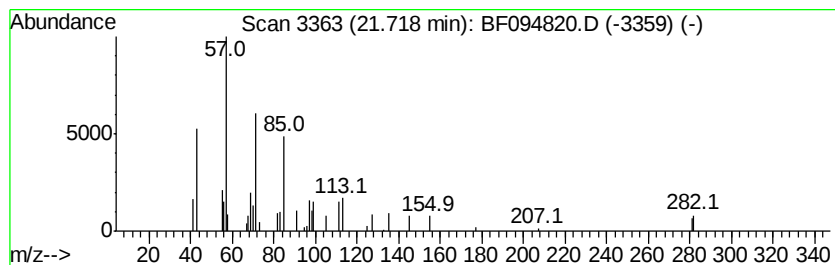
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.72	2.28 ng	50188	Perylene-d12	20.31

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	81
2	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	72
3	Heneicosane		296	C21H44	000629-94-7	59
4	Octadecane		254	C18H38	000593-45-3	59
5	Nonadecane		268	C19H40	000629-92-5	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050217\
Data File : BF094820.D
Acq On : 3 May 2017 6:44
Operator : SJ/MA
Sample : PB98658BL
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB98658BL

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
3-Penten-2-one, 4...	4.13	4.2	ng	114370	1	7.73	545863	20.0
2-Pentanone, 4-hy...	5.05	33.3	ng	908325	1	7.73	545863	20.0
unknown7.40	7.40	94.8	ng	2586380	1	7.73	545863	20.0
Heneicosane	20.79	2.7	ng	60436	6	20.31	441022	20.0
Hentriacontane	21.22	2.4	ng	53180	6	20.31	441022	20.0
Eicosane	21.72	2.3	ng	50188	6	20.31	441022	20.0