

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052217\
 Data File : BF095314.D
 Acq On : 22 May 2017 15:14
 Operator : SJ/MA
 Sample : I3210-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-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:\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	5.125	538	542	568	rBV	100969	265016	10.93%	1.413%
2	5.725	640	644	670	rBV	691668	1651694	68.14%	8.808%
3	7.295	908	911	928	rBV	853792	1615673	66.65%	8.616%
4	7.419	928	932	954	rVB	1150170	1989902	82.09%	10.611%
5	7.760	986	990	1000	rBV	305356	389213	16.06%	2.075%
6	7.995	1025	1030	1049	rBV	1120644	1456892	60.10%	7.769%
7	8.589	1127	1131	1137	rBV3	27862	69412	2.86%	0.370%
8	8.660	1139	1143	1178	rVB	569723	1184162	48.85%	6.315%
9	9.778	1329	1333	1355	rBV	353476	614742	25.36%	3.278%
10	10.936	1527	1530	1544	rBV3	10145	32949	1.36%	0.176%
11	11.548	1629	1634	1655	rBV	1571108	2424139	100.00%	12.927%
12	12.254	1750	1754	1770	rBV	141884	250375	10.33%	1.335%
13	12.613	1810	1815	1834	rBV2	449826	738010	30.44%	3.935%
14	13.442	1951	1956	1962	rBV	22210	26602	1.10%	0.142%
15	13.907	2030	2035	2061	rBV	718813	1374730	56.71%	7.331%
16	14.213	2083	2087	2091	rBV	19677	25928	1.07%	0.138%
17	15.013	2219	2223	2238	rBV	384194	688045	28.38%	3.669%
18	15.971	2381	2386	2400	rBV3	44452	103248	4.26%	0.551%
19	16.818	2527	2530	2538	rBV2	15352	25717	1.06%	0.137%
20	16.971	2545	2556	2562	rBV7	7213	25908	1.07%	0.138%
21	17.060	2567	2571	2576	rBV3	20228	34588	1.43%	0.184%
22	17.118	2576	2581	2588	rVB	20763	32208	1.33%	0.172%
23	17.330	2612	2617	2633	rBV	1844733	2235782	92.23%	11.922%
24	18.571	2823	2828	2843	rBV5	26712	82014	3.38%	0.437%
25	18.683	2843	2847	2866	rVB	331261	572606	23.62%	3.053%
26	19.353	2957	2961	2965	rBV	25574	30609	1.26%	0.163%
27	20.077	3080	3084	3089	rBV	204688	236350	9.75%	1.260%
28	20.359	3129	3132	3142	rBV	208703	384610	15.87%	2.051%
29	20.806	3203	3208	3214	rVB	62173	79396	3.28%	0.423%
30	21.136	3259	3264	3275	rBV6	43348	112240	4.63%	0.599%

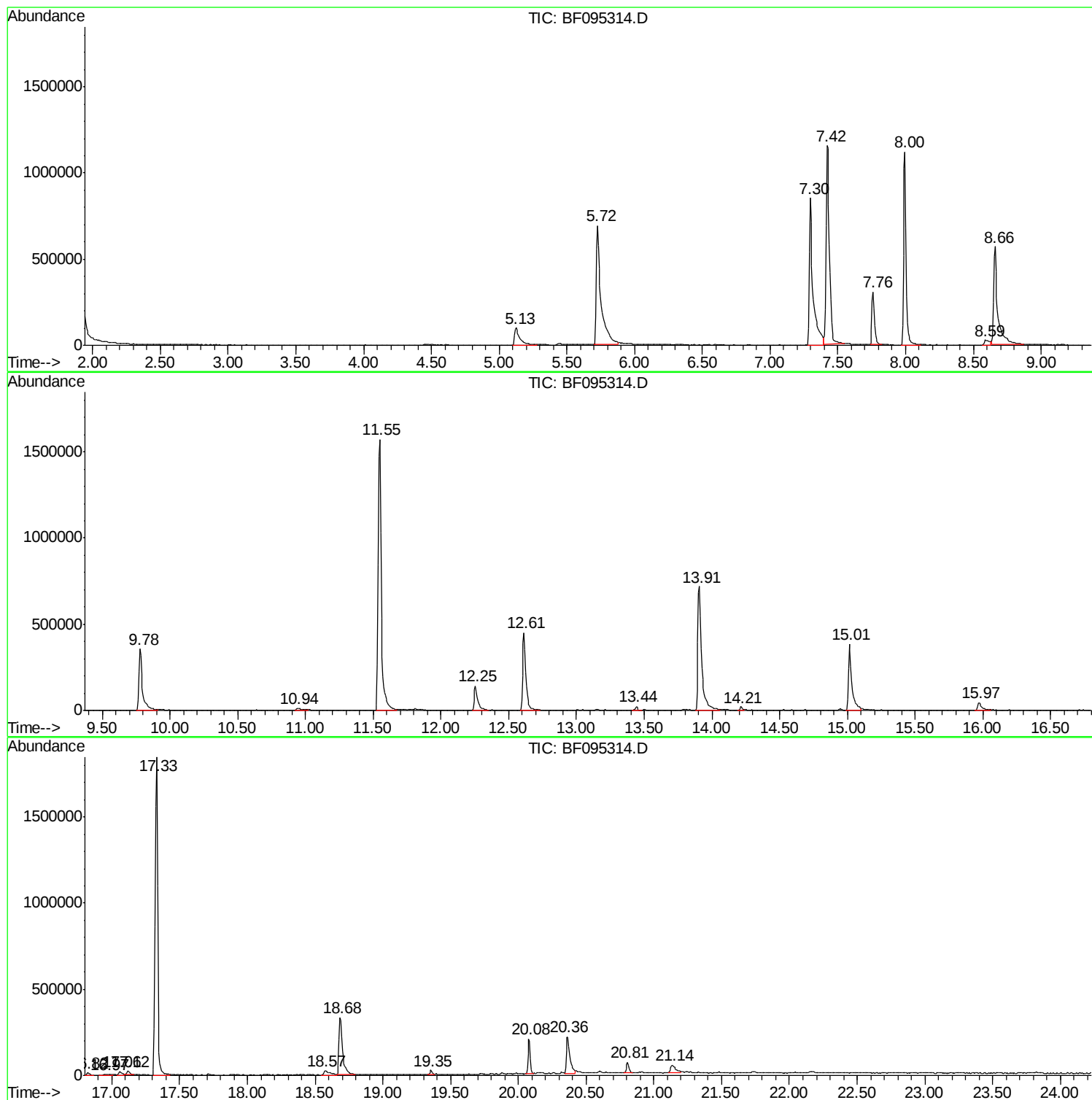
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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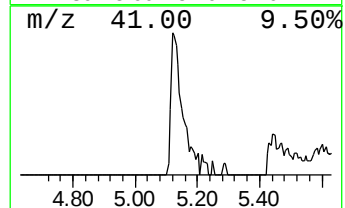
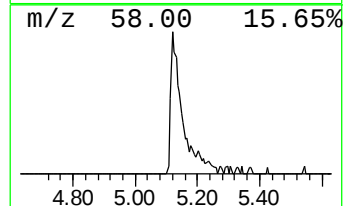
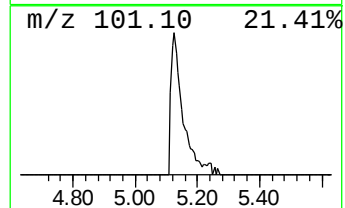
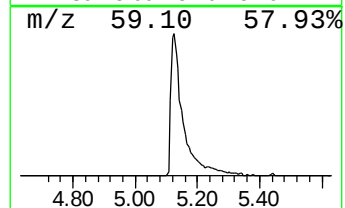
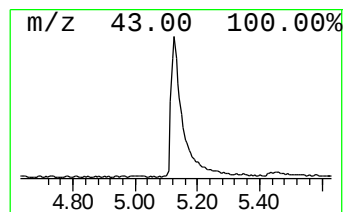
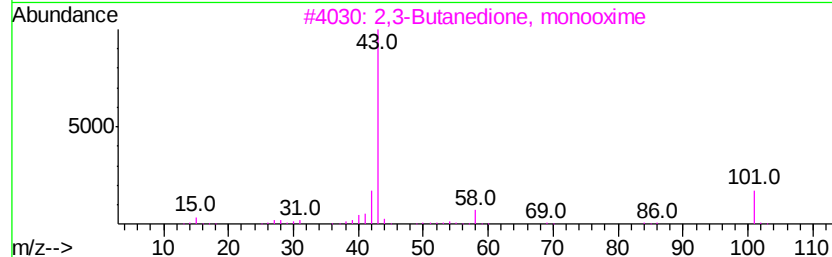
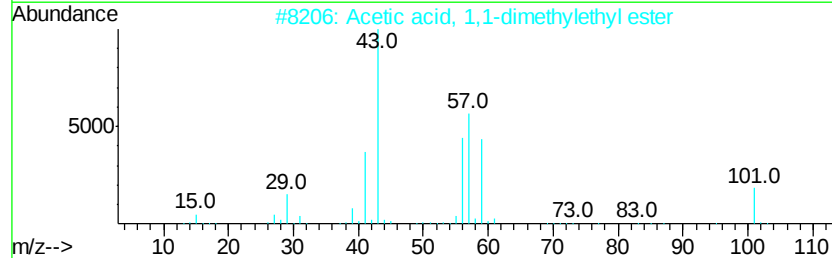
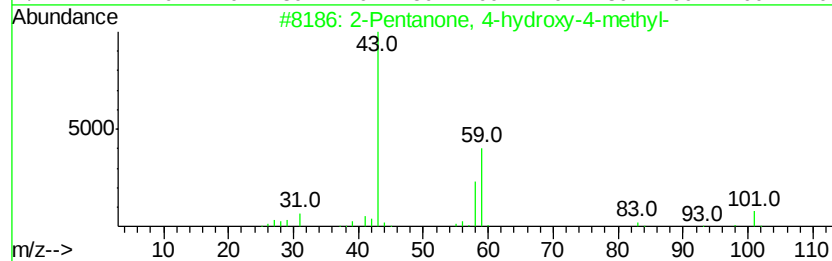
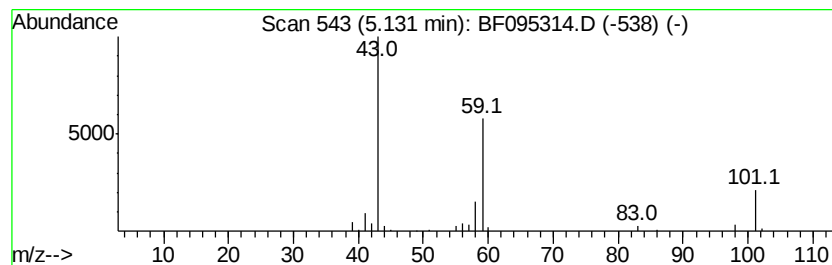
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	13.62 ng	265016	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
5		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17



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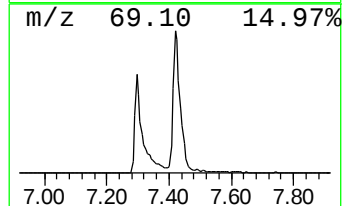
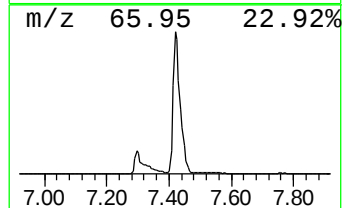
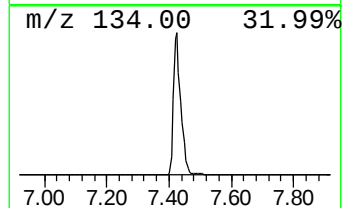
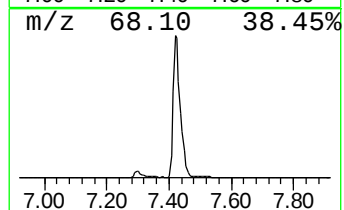
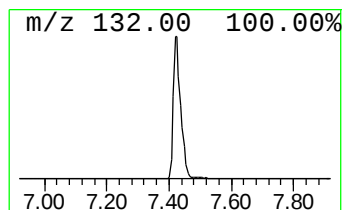
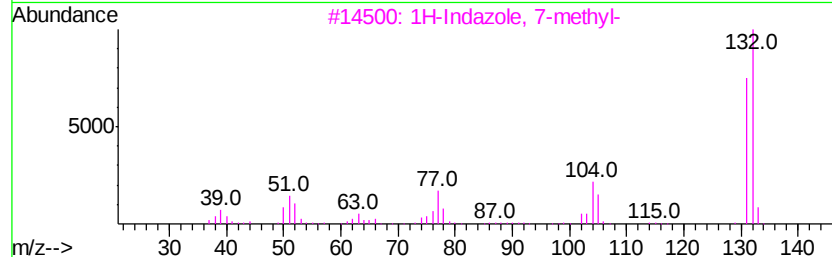
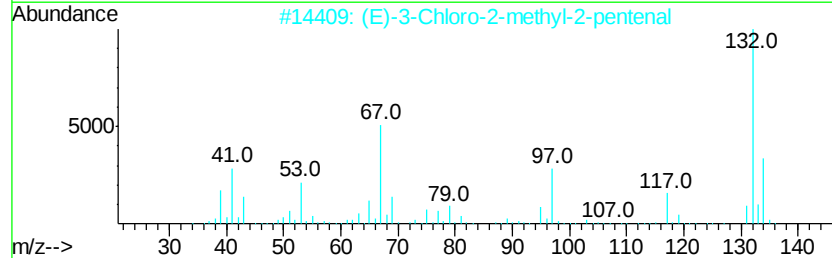
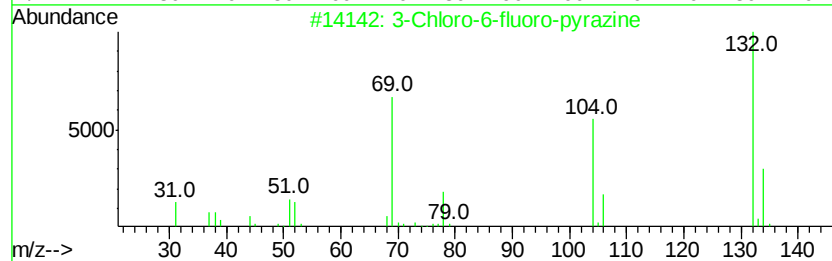
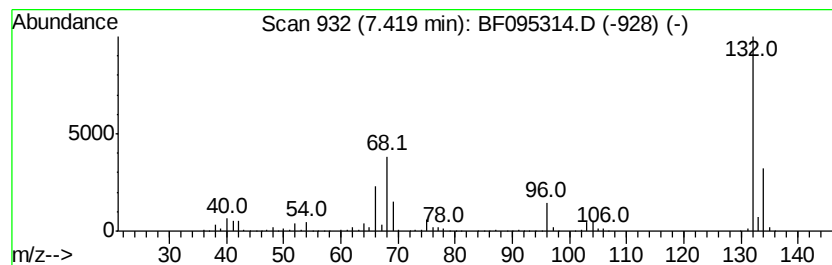
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Peak Number 2 unknown7.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.42	102.25 ng	1989900	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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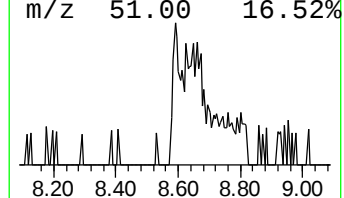
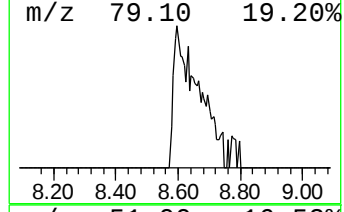
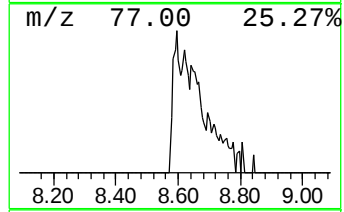
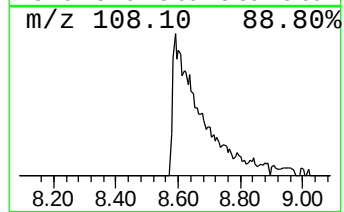
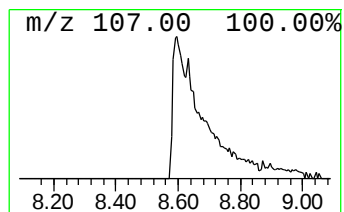
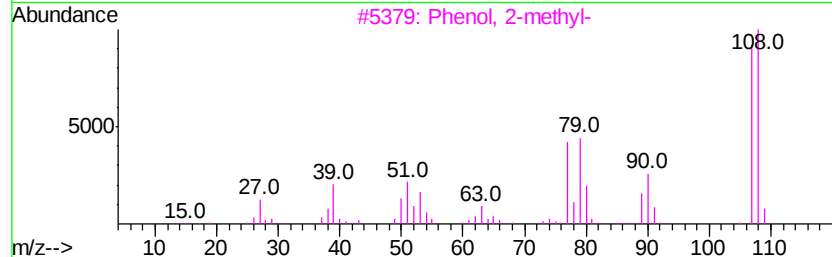
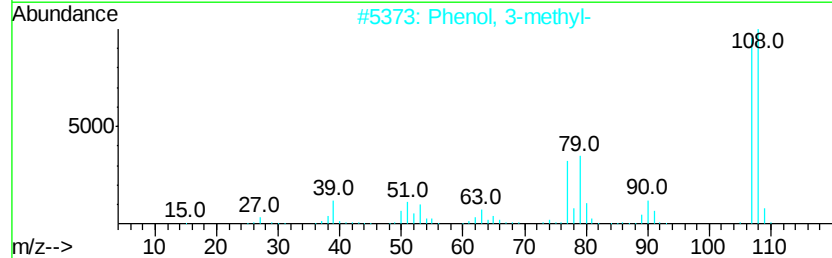
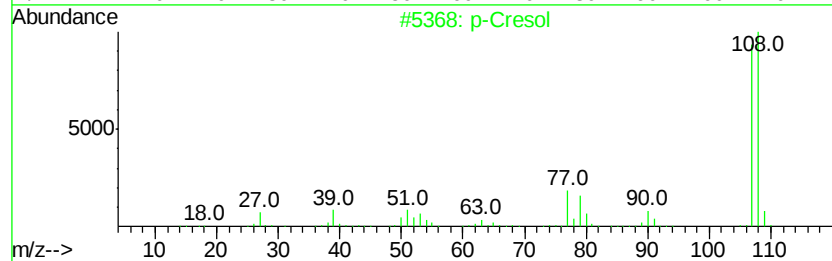
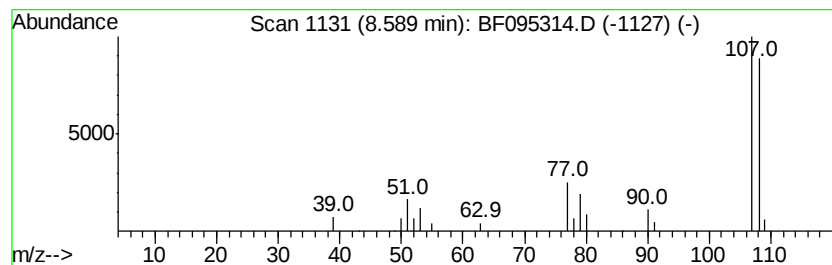
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Peak Number 4 p-Cresol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.59	3.57 ng	69412	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	p-Cresol	108	C7H8O	000106-44-5	95
2		Phenol, 3-methyl-	108	C7H8O	000108-39-4	72
3		Phenol, 2-methyl-	108	C7H8O	000095-48-7	64
4		o-Toluidine	107	C7H9N	000095-53-4	43
5		Carbamic acid, methyl-, 3-methyl...	165	C9H11NO2	001129-41-5	42



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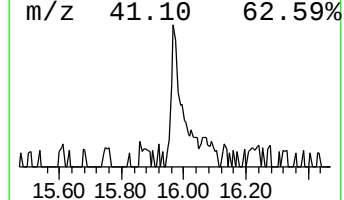
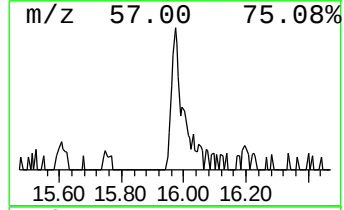
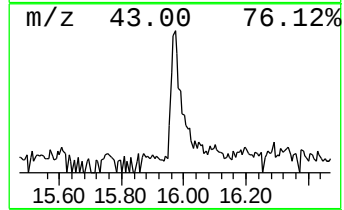
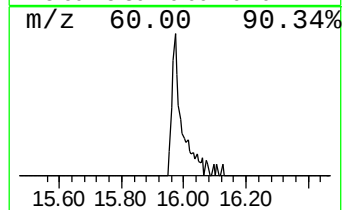
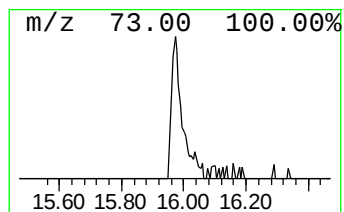
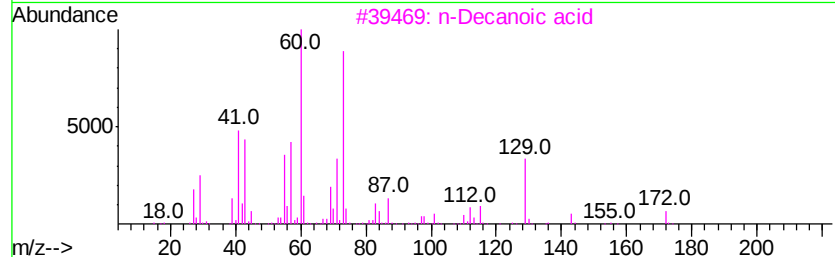
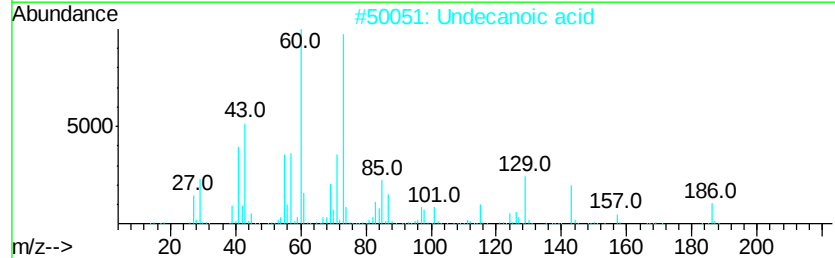
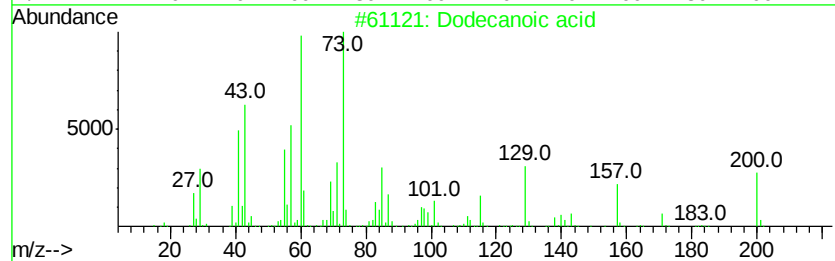
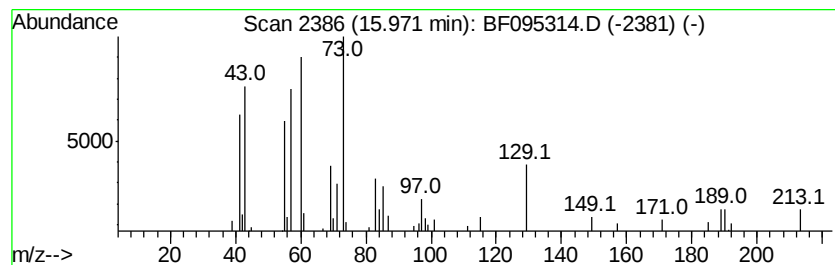
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Peak Number 5 Dodecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.97	3.00 ng	103248	Phenanthrene-d10		15.01

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	58
2			Undecanoic acid	186	C11H22O2	000112-37-8	47
3			n-Decanoic acid	172	C10H20O2	000334-48-5	47
4			Lactose	342	C12H22O11	000063-42-3	43
5			Nonanoic acid	158	C9H18O2	000112-05-0	38



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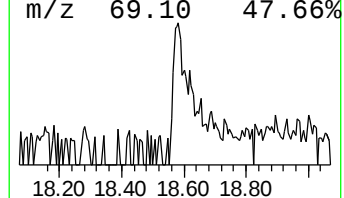
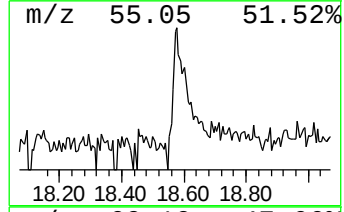
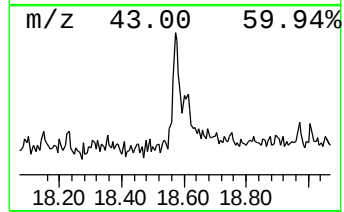
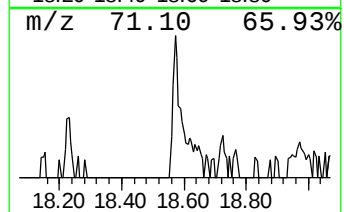
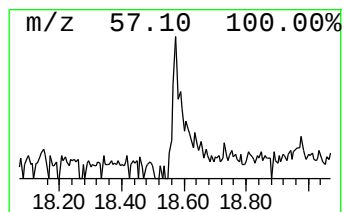
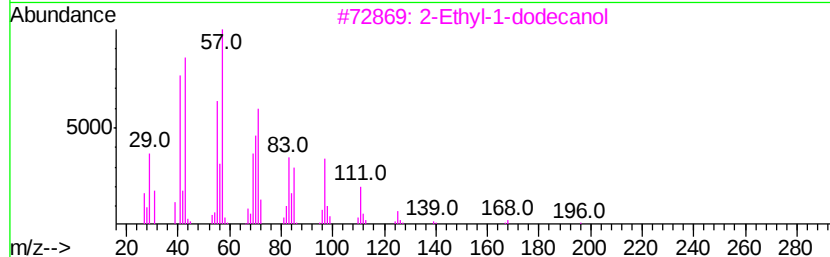
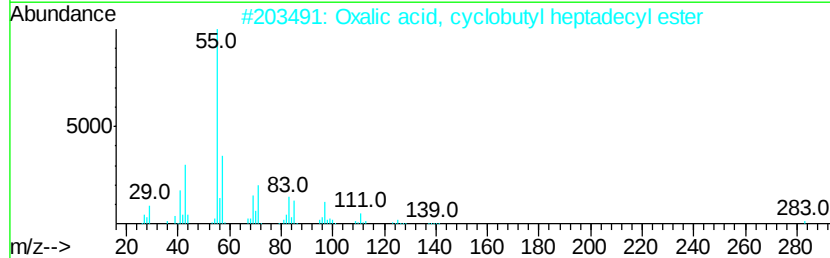
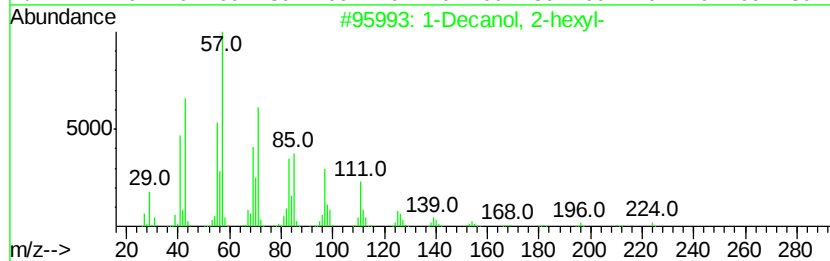
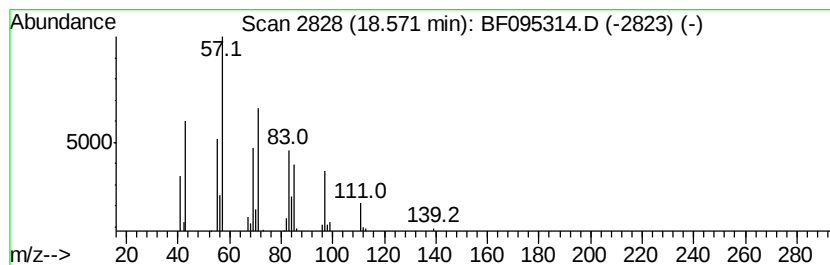
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 1-Decanol, 2-hexyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.57	2.86 ng	82014	Chrysene-d12	18.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	86
2		Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	72
3		2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	72
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	49
5		1-Docosene	308	C22H44	001599-67-3	49



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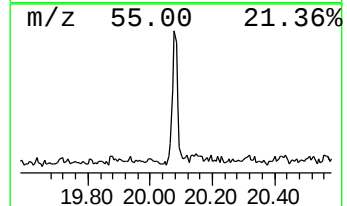
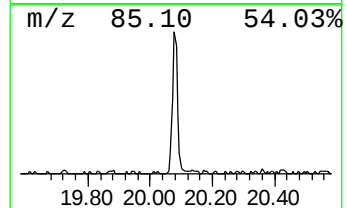
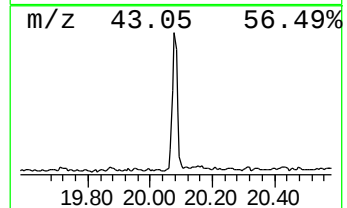
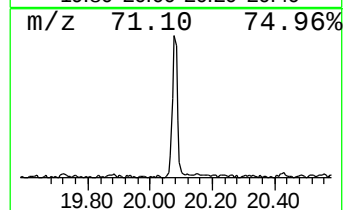
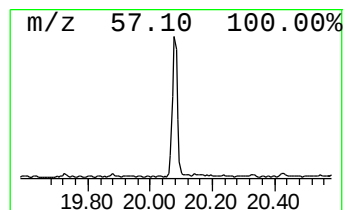
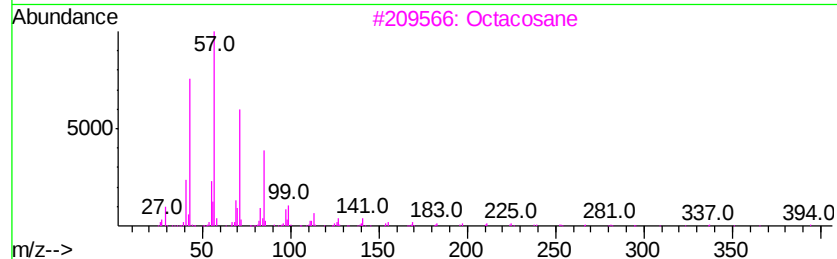
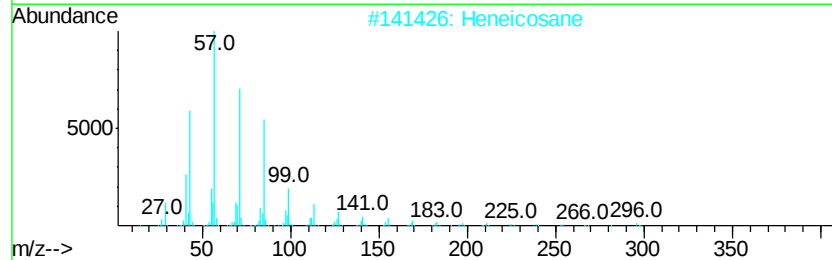
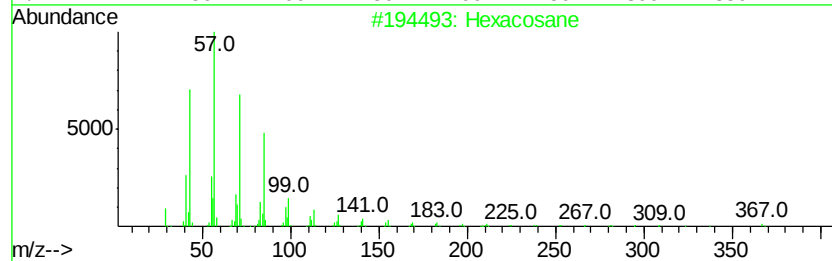
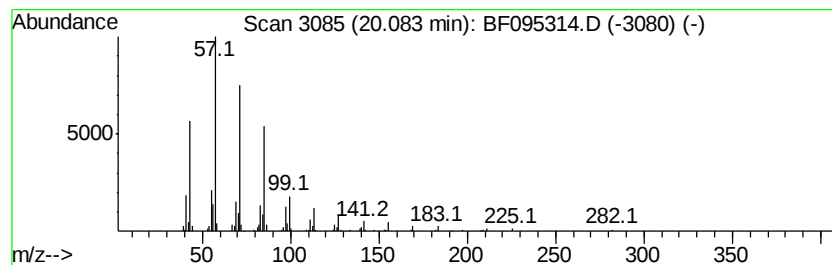
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.08	12.29 ng	236350	Perylene-d12	20.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	Octacosane		394	C28H58	000630-02-4	91
4	Heptacosane		380	C27H56	000593-49-7	91
5	2-methyloctacosane		408	C29H60	1000376-72-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052217\
Data File : BF095314.D
Acq On : 22 May 2017 15:14
Operator : SJ/MA
Sample : I3210-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-1

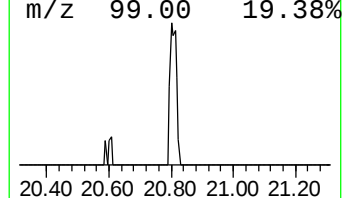
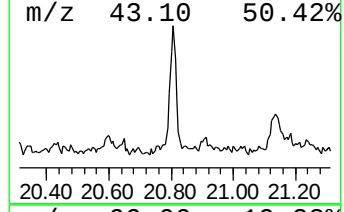
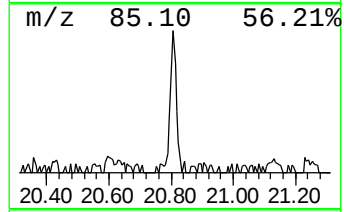
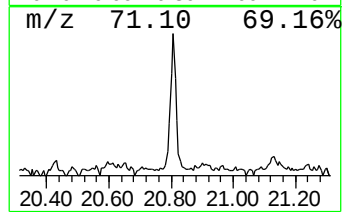
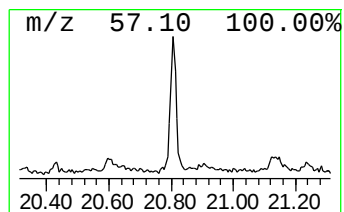
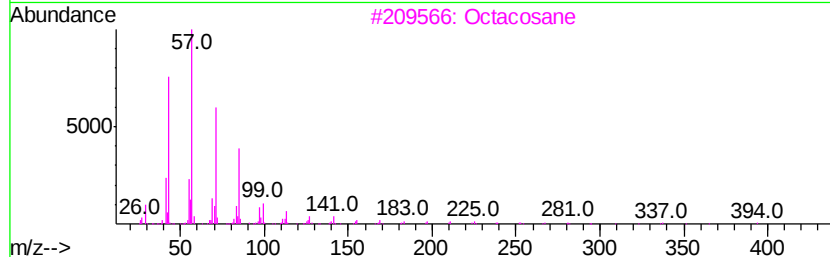
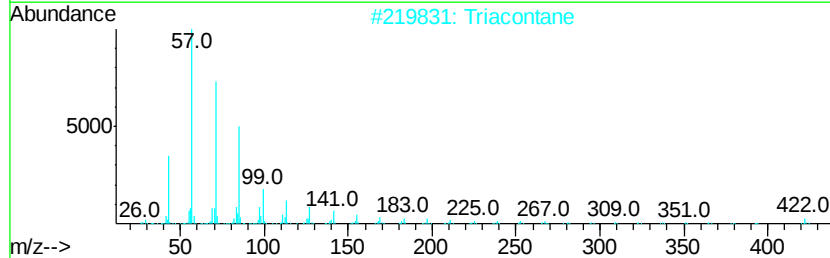
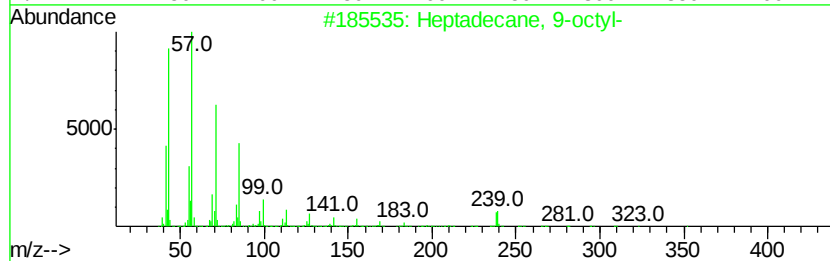
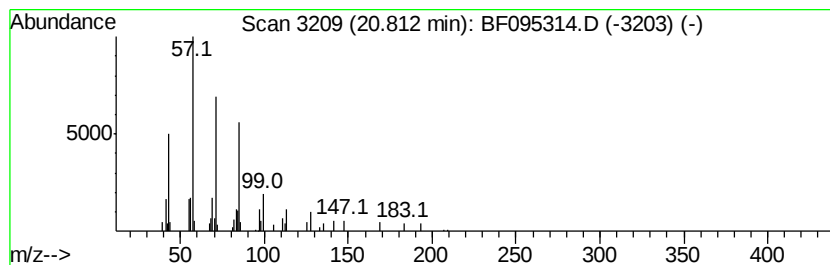
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.81	4.13 ng	79396	Perylene-d12	20.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		Triacontane	422	C30H62	000638-68-6	91
3		Octacosane	394	C28H58	000630-02-4	90
4		Heptacosane	380	C27H56	000593-49-7	90
5		Octadecane	254	C18H38	000593-45-3	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052217\
Data File : BF095314.D
Acq On : 22 May 2017 15:14
Operator : SJ/MA
Sample : I3210-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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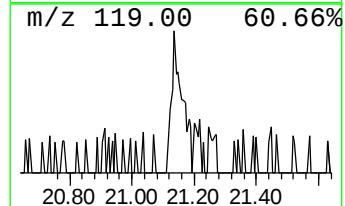
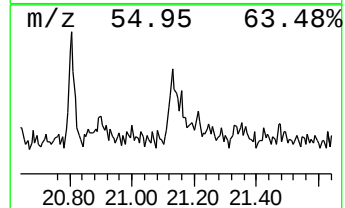
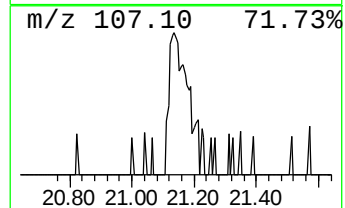
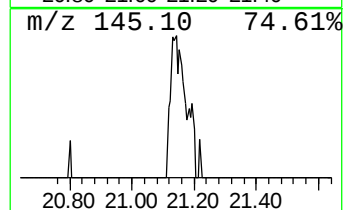
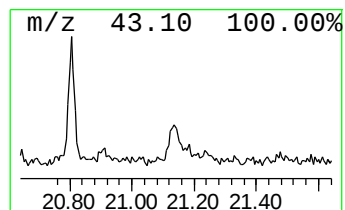
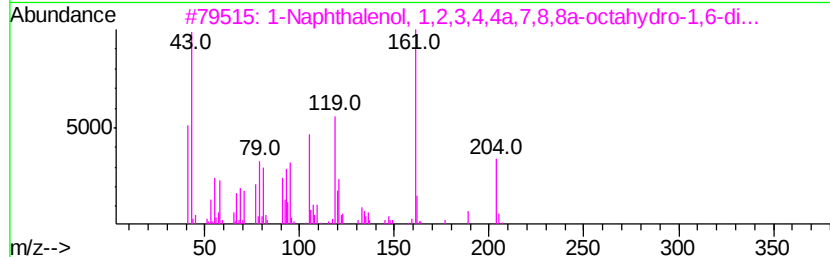
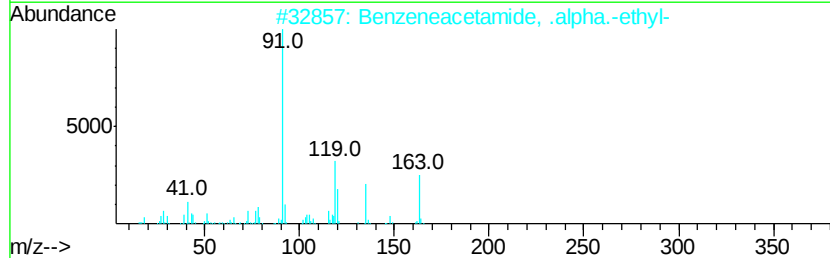
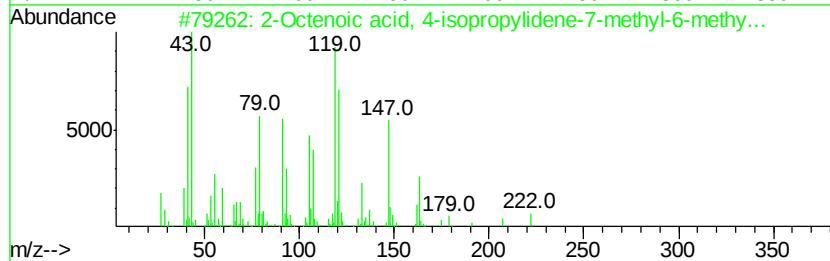
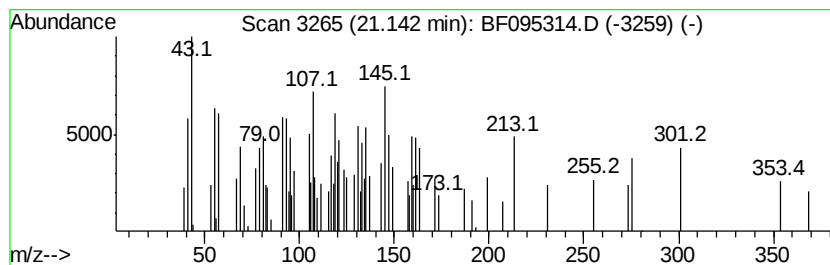
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown21.14 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.14	5.84 ng	112240	Perylene-d12	20.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Octenoic acid, 4-isopropyliden...	222	C14H22O2	1000151-99-2	22
2		Benzeneacetamide, .alpha.-ethyl-	163	C10H13NO	000090-26-6	18
3		1-Naphthalenol, 1,2,3,4,4a,7,8,8...	222	C15H26O	019435-97-3	14
4		2-(4-(But-2-yl)phenyl)propanoic ...	206	C13H18O2	064451-76-9	10
5		1,6-Cyclodecadiene, 1-methyl-5-m...	204	C15H24	023986-74-5	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052217\
Data File : BF095314.D
Acq On : 22 May 2017 15:14
Operator : SJ/MA
Sample : I3210-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.13	13.6	ng	265016	1	7.76	389213	20.0
unknown7.42	7.42	102.3	ng	1989900	1	7.76	389213	20.0
p-Cresol	8.59	3.6	ng	69412	1	7.76	389213	20.0
Dodecanoic acid	15.97	3.0	ng	103248	4	15.01	688045	20.0
1-Decanol, 2-hexyl-	18.57	2.9	ng	82014	5	18.68	572606	20.0
Hexacosane	20.08	12.3	ng	236350	6	20.36	384610	20.0
Heptadecane, 9-oc...	20.81	4.1	ng	79396	6	20.36	384610	20.0
unknown21.14	21.14	5.8	ng	112240	6	20.36	384610	20.0