

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
 Data File : BF095567.D
 Acq On : 31 May 2017 16:55
 Operator : SJ/MA
 Sample : I3329-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-14(6-9)

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	4.819	503	507	526	rBV	90976	271891	7.18%	0.856%
2	5.472	614	618	653	rBV	1679010	2994354	79.08%	9.432%
3	7.107	890	896	909	rBV	1833708	2997732	79.17%	9.443%
4	7.213	909	914	934	rVB	2321994	3350054	88.47%	10.552%
5	7.548	967	971	982	rBV	417606	581053	15.35%	1.830%
6	7.789	1007	1012	1038	rVB	1802216	2471059	65.26%	7.784%
7	8.466	1122	1127	1157	rBV	1326759	2003295	52.91%	6.310%
8	9.583	1312	1317	1332	rBV	600774	852169	22.51%	2.684%
9	11.360	1612	1619	1632	rBV	2637296	3786463	100.00%	11.927%
10	12.048	1732	1736	1748	rBV	467250	593093	15.66%	1.868%
11	12.407	1792	1797	1806	rBV2	681353	903874	23.87%	2.847%
12	13.254	1936	1941	1945	rBV	35190	40149	1.06%	0.126%
13	13.707	2012	2018	2033	rBV	1464587	2195865	57.99%	6.917%
14	14.024	2067	2072	2083	rBV	60800	93105	2.46%	0.293%
15	14.754	2192	2196	2200	rBV	34629	40589	1.07%	0.128%
16	14.807	2200	2205	2209	rVV2	734813	943219	24.91%	2.971%
17	14.848	2209	2212	2223	rVB	158904	246212	6.50%	0.776%
18	14.954	2226	2230	2237	rBV	30821	47858	1.26%	0.151%
19	15.795	2370	2373	2385	rVB2	148360	204441	5.40%	0.644%
20	16.612	2508	2512	2518	rBV	283621	334693	8.84%	1.054%
21	16.912	2557	2563	2570	rBV	290916	417015	11.01%	1.314%
22	17.165	2599	2606	2609	rBV	2492154	3317000	87.60%	10.448%
23	17.524	2663	2667	2676	rBV5	32204	68087	1.80%	0.214%
24	18.401	2812	2816	2826	rVB3	140852	239376	6.32%	0.754%
25	18.506	2828	2834	2838	rBV2	665084	882250	23.30%	2.779%
26	18.542	2838	2840	2847	rVB2	73821	112552	2.97%	0.355%
27	19.212	2950	2954	2958	rBV4	44254	62269	1.64%	0.196%
28	19.306	2967	2970	2978	rVB2	34254	69844	1.84%	0.220%
29	19.395	2982	2985	2987	rVV2	44046	50144	1.32%	0.158%
30	19.430	2988	2991	2994	rVB	48835	57335	1.51%	0.181%
31	19.495	2999	3002	3005	rVV	56596	73148	1.93%	0.230%
32	19.530	3005	3008	3014	rVV3	82030	102683	2.71%	0.323%
33	19.589	3015	3018	3022	rVV	47196	60717	1.60%	0.191%
34	19.636	3022	3026	3031	rVB3	50068	70751	1.87%	0.223%

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35	19.689	3031	3035	3039	rBV2	31977	39505	1.04%	0.124%
36	19.783	3047	3051	3054	rBV	95513	133038	3.51%	0.419%
37	20.071	3097	3100	3104	rVB	54251	53544	1.41%	0.169%
38	20.130	3106	3110	3114	rVV	90218	104047	2.75%	0.328%
39	20.177	3114	3118	3127	rVB	500025	656642	17.34%	2.068%
40	20.677	3197	3203	3214	rVB	34394	102386	2.70%	0.323%
41	21.441	3329	3333	3342	rBV3	26726	58376	1.54%	0.184%
42	21.806	3390	3395	3405	rBV2	27261	65201	1.72%	0.205%

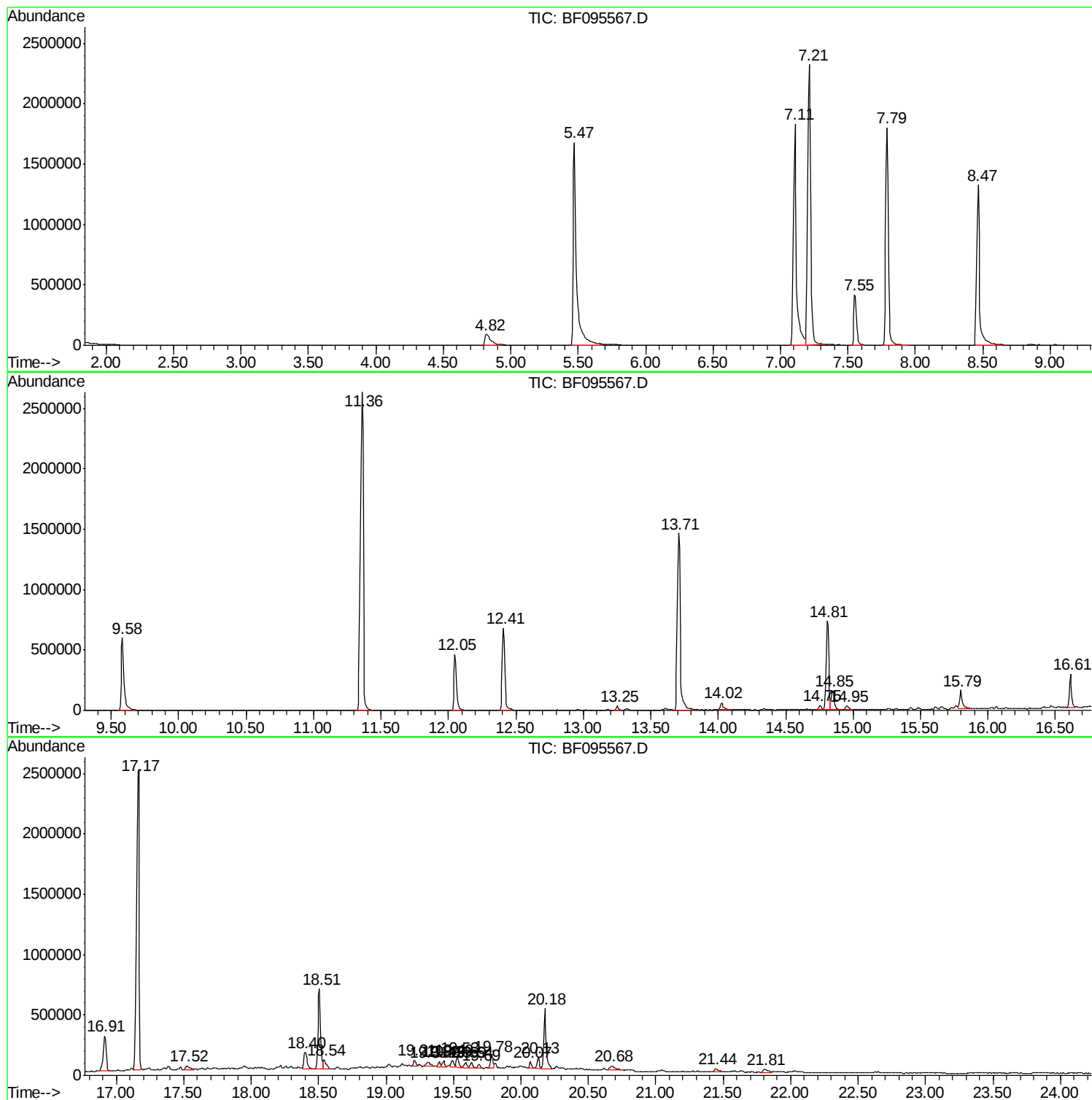
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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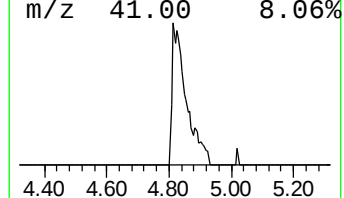
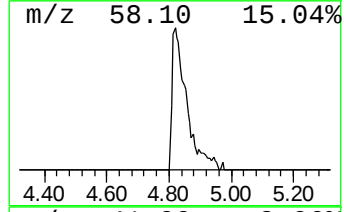
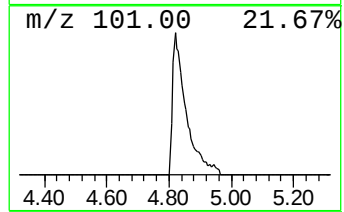
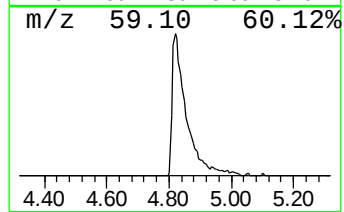
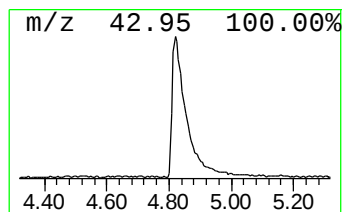
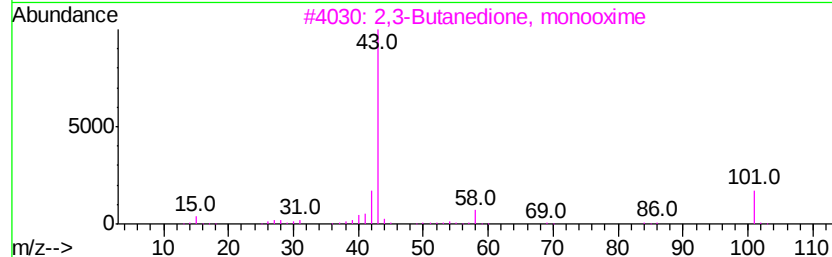
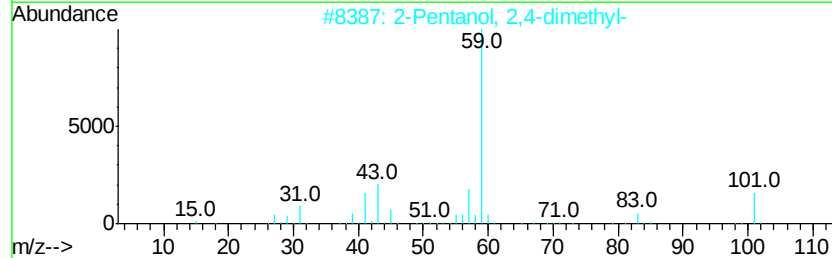
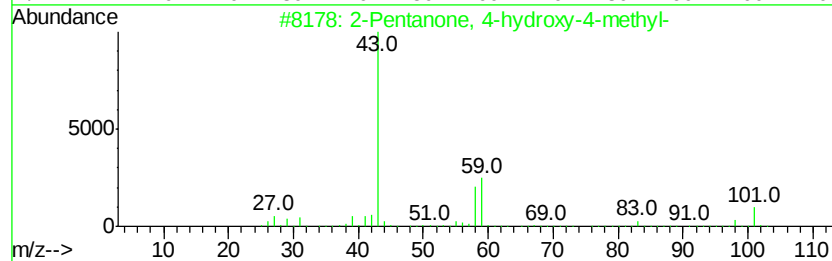
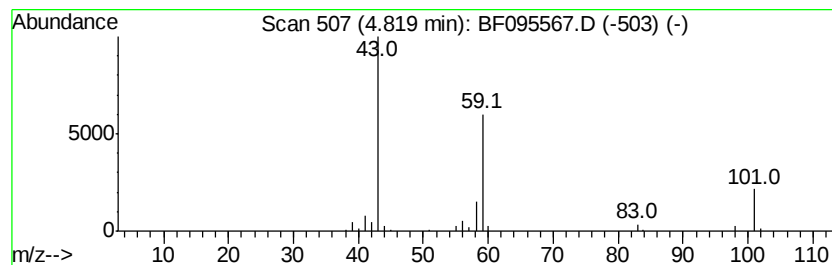
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.82	9.36 ng	271891	1,4-Dichlorobenzene-d4	7.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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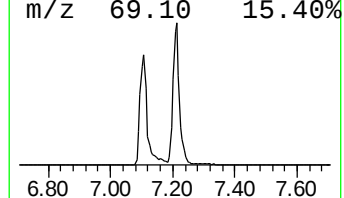
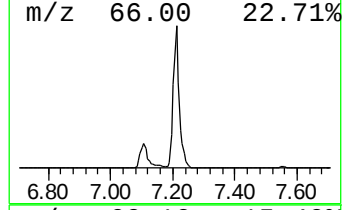
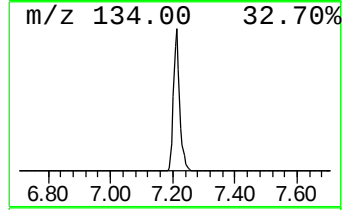
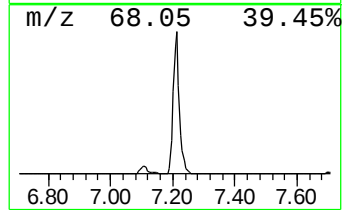
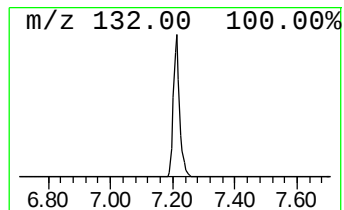
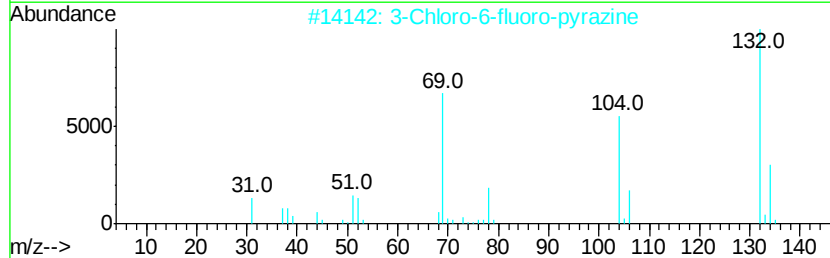
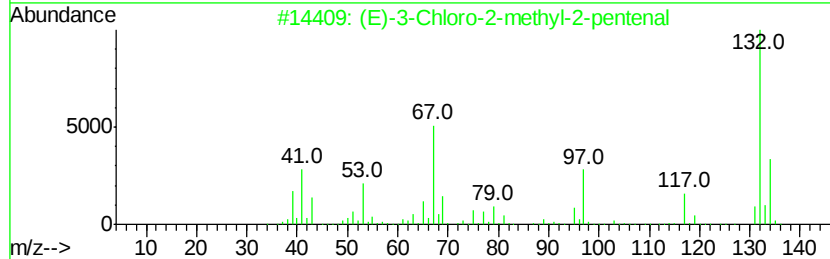
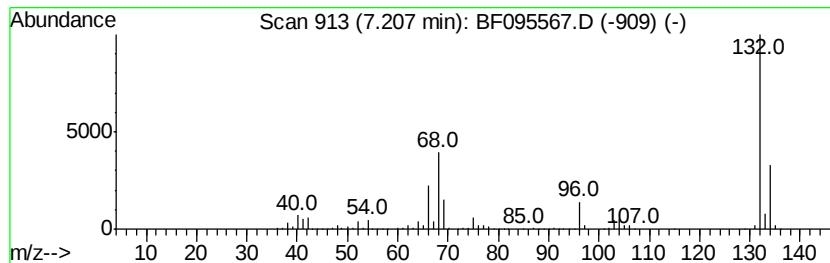
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	115.31 ng	3350050	1,4-Dichlorobenzene-d4	7.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10



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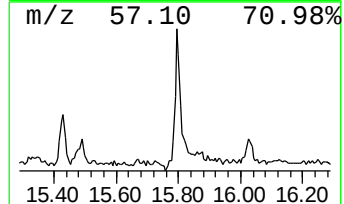
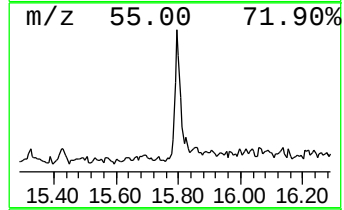
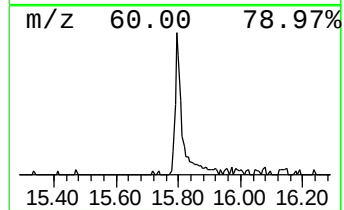
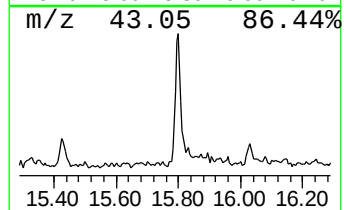
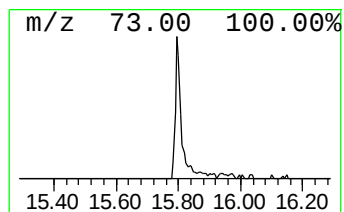
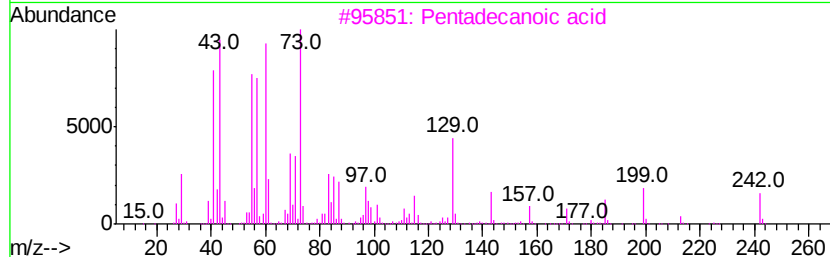
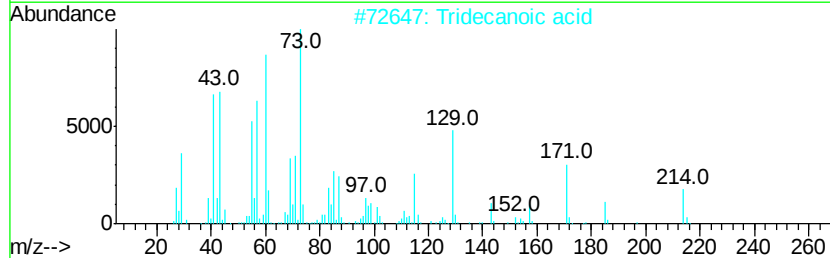
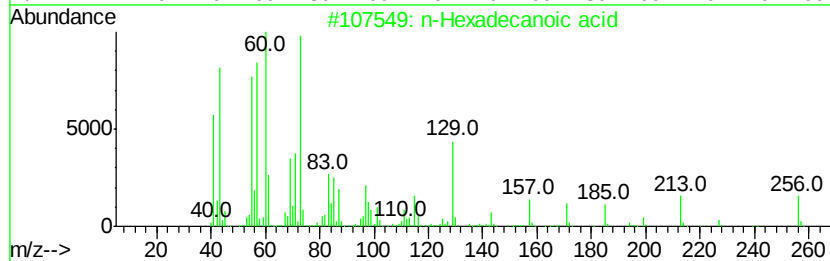
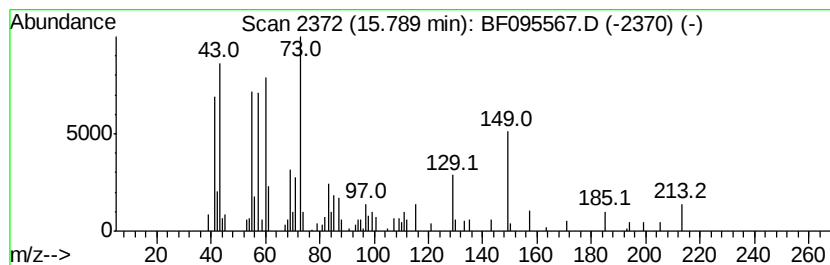
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.79	4.33 ng	204441	Phenanthrene-d10	14.81	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	49



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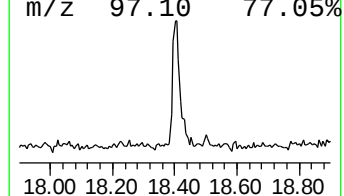
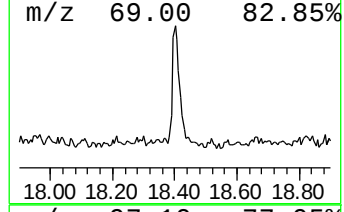
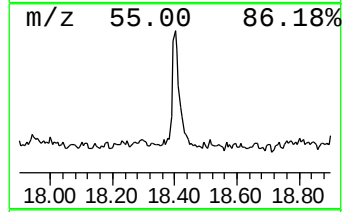
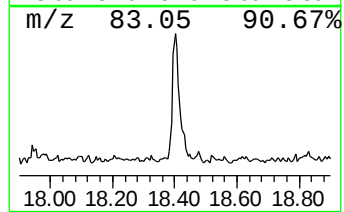
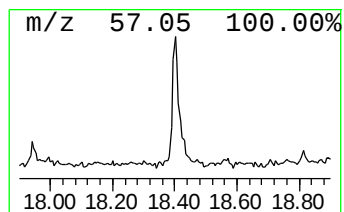
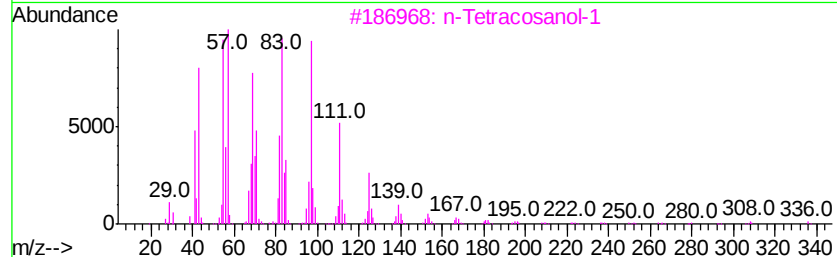
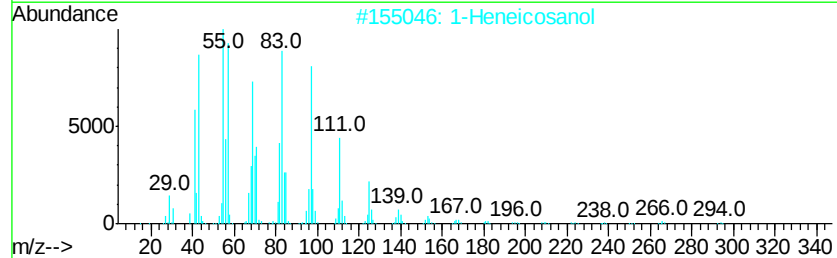
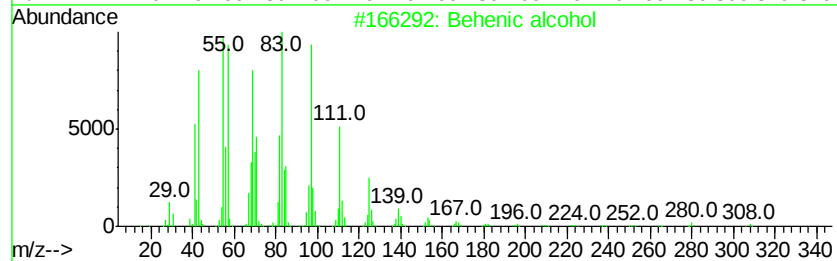
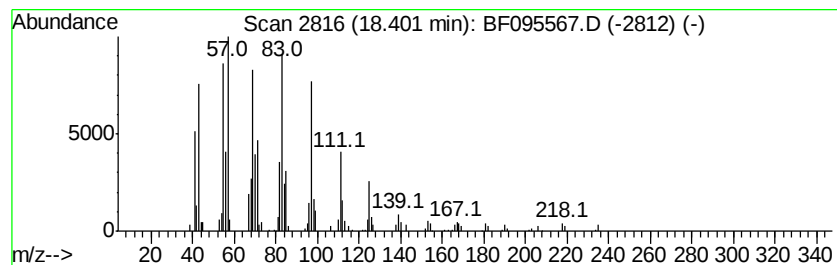
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.40	5.43 ng	239376	Chrysene-d12	18.51
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Behenic alcohol	326 C22H46O	000661-19-8 95
2		1-Heneicosanol	312 C21H44O	015594-90-8 95
3		n-Tetracosanol-1	354 C24H50O	000506-51-4 93
4		Heptadecyl trifluoroacetate	352 C19H35F3O2	1000351-87-0 93
5		Trichloroacetic acid, pentadecyl...	372 C17H31Cl3O2	074339-53-0 91



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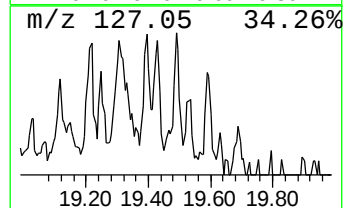
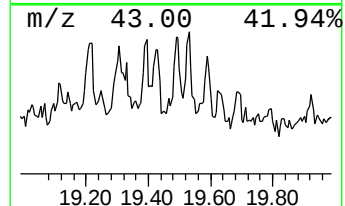
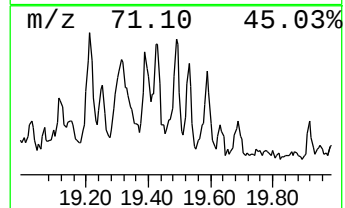
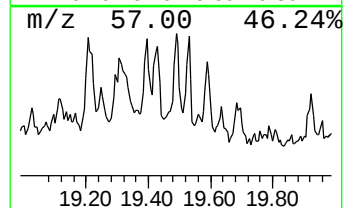
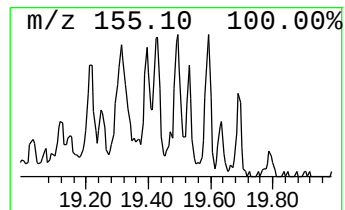
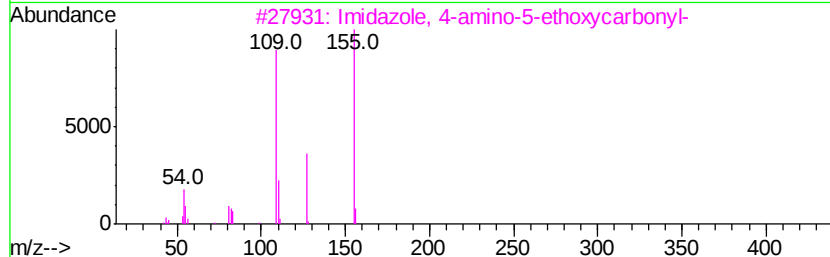
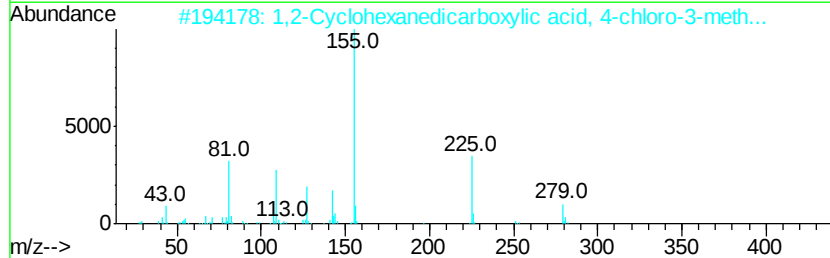
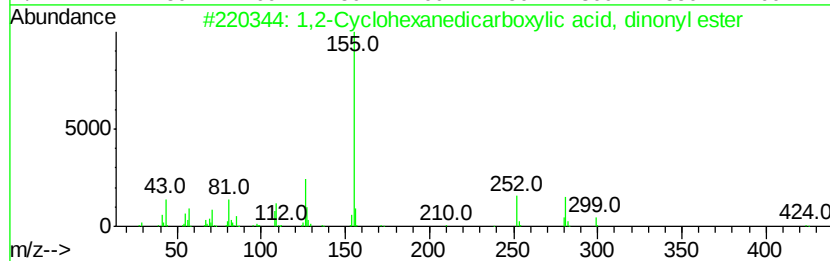
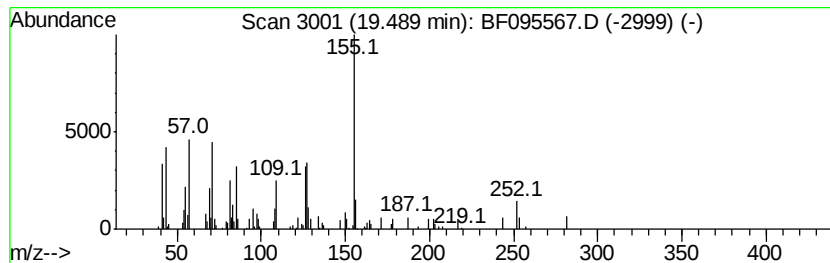
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Peak Number 6 unknown19.49 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.49	2.23 ng	73148	Perylene-d12	20.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Cyclohexanedicarboxylic acid...	424	C26H48O4	1000339-40-5	47
2		1,2-Cyclohexanedicarboxylic acid...	366	C20H27ClO4	1000339-68-7	47
3		Imidazole, 4-amino-5-ethoxycarbo...	155	C6H9N3O2	021190-16-9	43
4		1,2-Cyclohexanedicarboxylic acid...	324	C19H32O4	1000339-75-3	43
5		1,2-Cyclohexanedicarboxylic acid...	350	C20H27FO4	1000339-78-4	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053117\
Data File : BF095567.D
Acq On : 31 May 2017 16:55
Operator : SJ/MA
Sample : I3329-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-14(6-9)

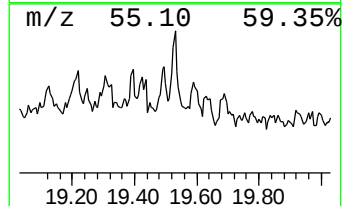
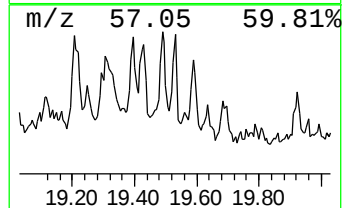
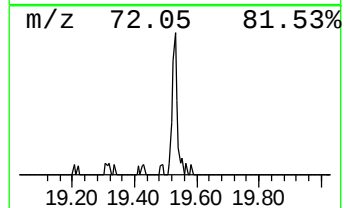
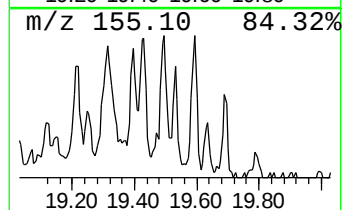
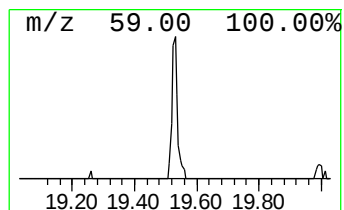
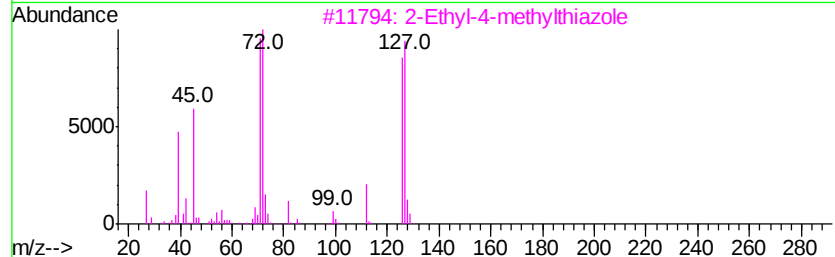
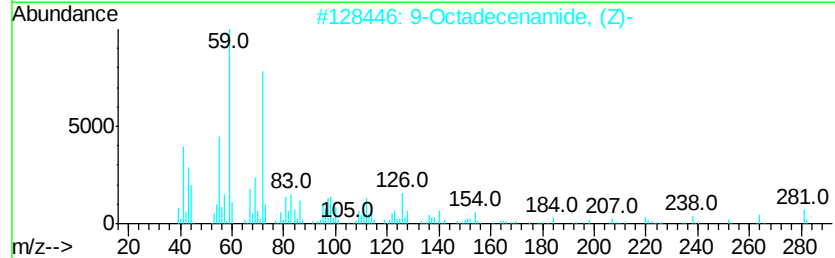
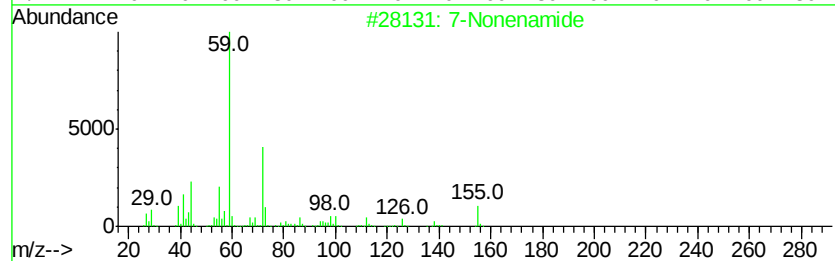
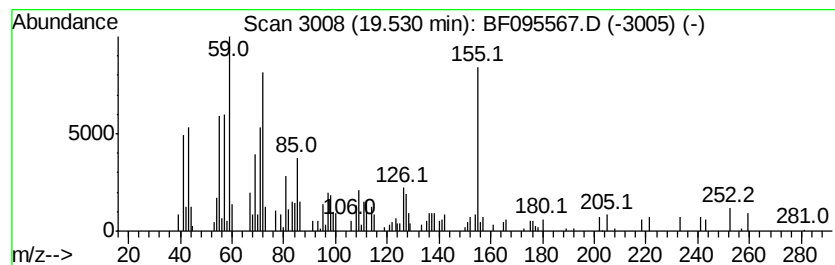
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 7-Nonenamide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.53	3.13 ng	102683	Perylene-d12	20.18

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Nonenamide		155	C9H17NO	090949-53-4	50
2	9-Octadecenamide, (Z)-		281	C18H35NO	000301-02-0	43
3	2-Ethyl-4-methylthiazole		127	C6H9NS	015679-12-6	22
4	Dodecanamide		199	C12H25NO	001120-16-7	22
5	Butanal, 2-ethyl-		100	C6H12O	000097-96-1	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053117\
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Acq On : 31 May 2017 16:55
Operator : SJ/MA
Sample : I3329-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-14(6-9)

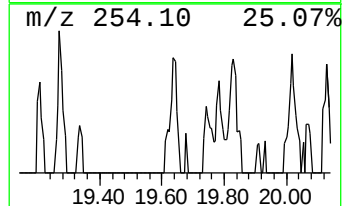
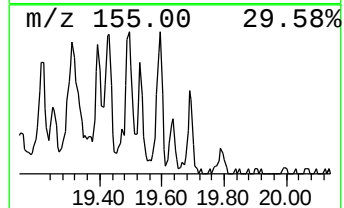
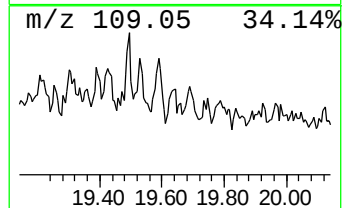
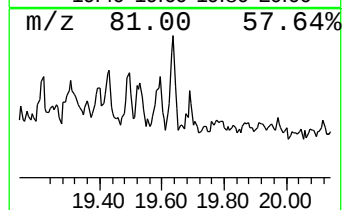
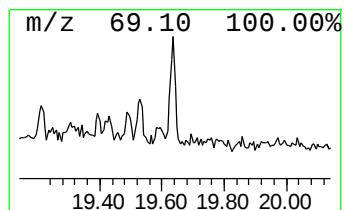
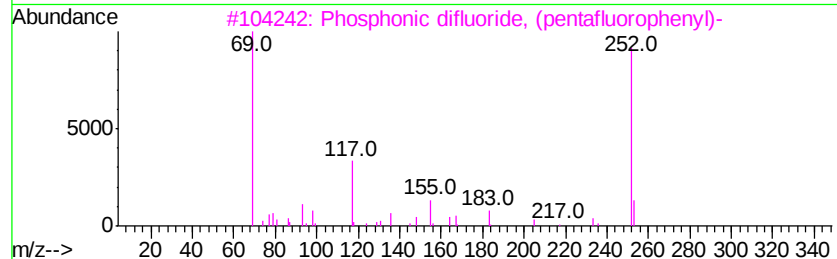
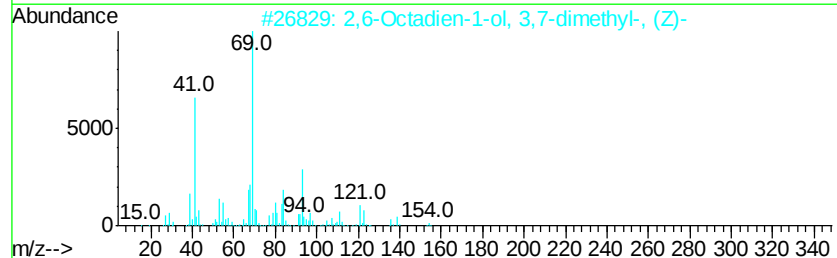
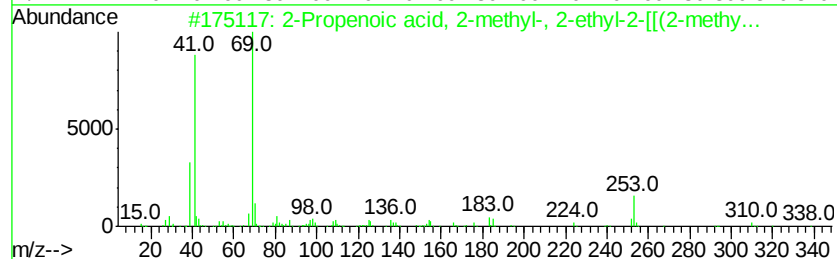
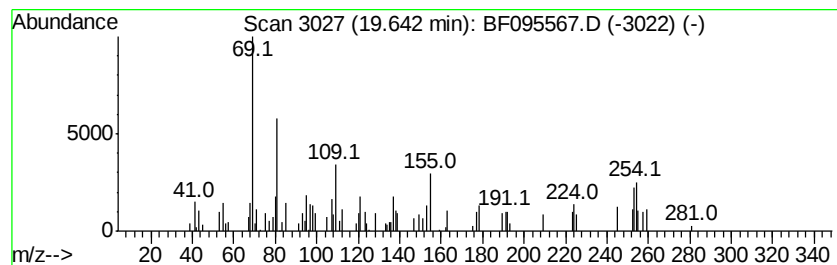
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown19.64 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.64	2.15 ng	70751	Perylene-d12	20.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propenoic acid, 2-methyl-, 2-e...	338	C18H26O6	003290-92-4	38
2		2,6-Octadien-1-ol, 3,7-dimethyl-...	154	C10H18O	000106-25-2	38
3		Phosphonic difluoride, (pentaflu...	252	C6F7OP	022474-68-6	38
4		Squalene	410	C30H50	000111-02-4	35
5		4-Hexen-3-one, 2,2-dimethyl-	126	C8H14O	020971-19-1	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095567.D
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Operator : SJ/MA
Sample : I3329-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-14(6-9)

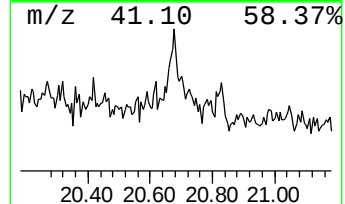
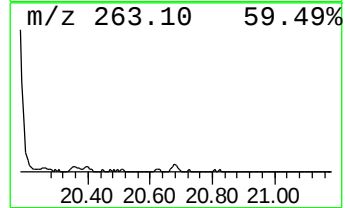
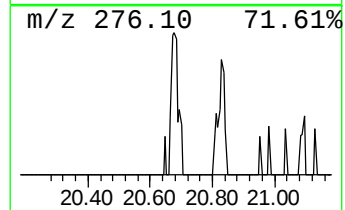
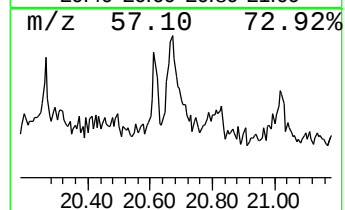
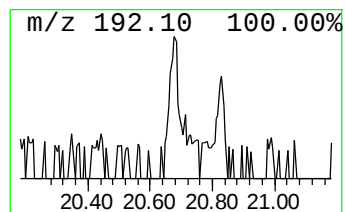
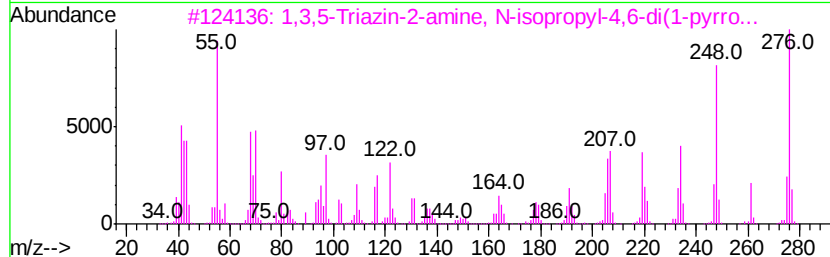
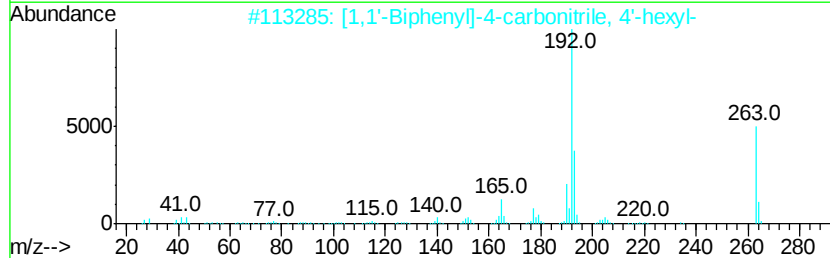
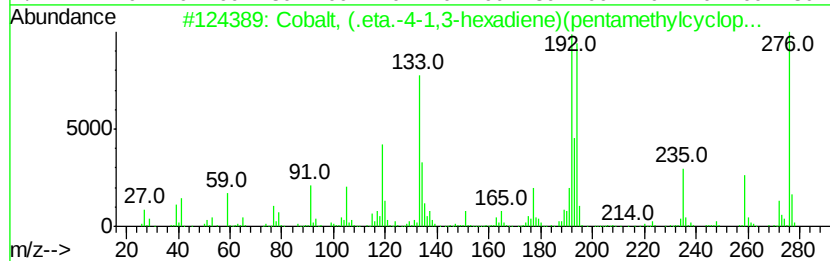
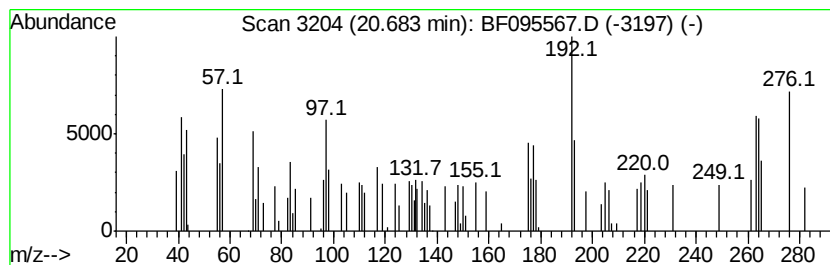
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cobalt, (.eta.-4-1,3-hexadi... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.68	3.12 ng	102386	Perylene-d12	20.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cobalt, (.eta.-4-1,3-hexadiene)(...	276	C16H25Co	1000156-29-9	50
2		[1,1'-Biphenyl]-4-carbonitrile, ...	263	C19H21N	041122-70-7	30
3		1,3,5-Triazin-2-amine, N-isoprop...	276	C14H24N6	1000276-80-0	25
4		Cyclopentane-1-carboxylic acid, ...	252	C14H20O4	1000159-41-3	14
5		Dodecahydropyrido[1,2-b]isoquino...	193	C13H23N	113039-29-5	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053117\
Data File : BF095567.D
Acq On : 31 May 2017 16:55
Operator : SJ/MA
Sample : I3329-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-14(6-9)

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...	4.82	9.4	ng	271891	1	7.55	581053	20.0
unknown7.21	7.21	115.3	ng	3350050	1	7.55	581053	20.0
n-Hexadecanoic acid	15.79	4.3	ng	204441	4	14.81	943219	20.0
Behenic alcohol	18.40	5.4	ng	239376	5	18.51	882250	20.0
unknown19.49	19.49	2.2	ng	73148	6	20.18	656642	20.0
7-Nonenamide	19.53	3.1	ng	102683	6	20.18	656642	20.0
unknown19.64	19.64	2.1	ng	70751	6	20.18	656642	20.0
Cobalt, (.eta.-4-...	20.68	3.1	ng	102386	6	20.18	656642	20.0