

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061116\
 Data File : BF087935.D
 Acq On : 12 Jun 2016 8:17
 Operator : UM/SJ
 Sample : H3504-03
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-3

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-BF060716.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	1.735	12	13	22	rVB	244548	374232	11.05%	1.347%
2	1.861	22	24	37	rVB	1946345	3123937	92.24%	11.246%
3	4.958	293	295	303	rVB	91547	116644	3.44%	0.420%
4	5.393	330	333	335	rVB	1300421	1481889	43.75%	5.335%
5	6.433	421	424	426	rBV	989631	1044027	30.83%	3.759%
6	6.570	433	436	438	rBV	2181507	2542709	75.08%	9.154%
7	6.799	454	456	458	rBV	787538	648435	19.15%	2.334%
8	6.959	467	470	472	rBV	2290878	2201690	65.01%	7.926%
9	7.370	503	506	508	rBV	1779140	1986151	58.64%	7.150%
10	8.090	566	569	571	rBV	873209	873805	25.80%	3.146%
11	9.165	660	663	666	rBV	2604621	3386789	100.00%	12.193%
12	9.565	695	698	700	rBV	167393	177835	5.25%	0.640%
13	9.839	720	722	725	rBV	1068546	992439	29.30%	3.573%
14	10.353	765	767	769	rVB	50889	41852	1.24%	0.151%
15	10.628	788	791	794	rBV	1751809	1967097	58.08%	7.082%
16	10.730	798	800	801	rBV	41030	47809	1.41%	0.172%
17	11.199	838	841	843	rBV2	52380	56762	1.68%	0.204%
18	11.325	849	852	854	rVV	956363	1001305	29.57%	3.605%
19	11.565	870	873	876	rVV	98610	158146	4.67%	0.569%
20	11.622	876	878	881	rVB	48731	47170	1.39%	0.170%
21	12.034	912	914	916	rBV	54940	57456	1.70%	0.207%
22	12.376	942	944	947	rBV	349091	377704	11.15%	1.360%
23	12.742	973	976	977	rBV	107484	103352	3.05%	0.372%
24	12.788	977	980	988	rVB3	24052	63695	1.88%	0.229%
25	12.914	988	991	993	rBV	2696724	2864761	84.59%	10.313%
26	13.359	1028	1030	1036	rBV	68015	95498	2.82%	0.344%
27	13.451	1036	1038	1043	rBV3	98202	183850	5.43%	0.662%
28	13.817	1067	1070	1075	rBV	95961	118616	3.50%	0.427%
29	13.954	1079	1082	1085	rBV	1000090	969080	28.61%	3.489%
30	14.811	1154	1157	1164	rVB2	22473	44671	1.32%	0.161%
31	15.371	1203	1206	1209	rBV	459918	627884	18.54%	2.260%

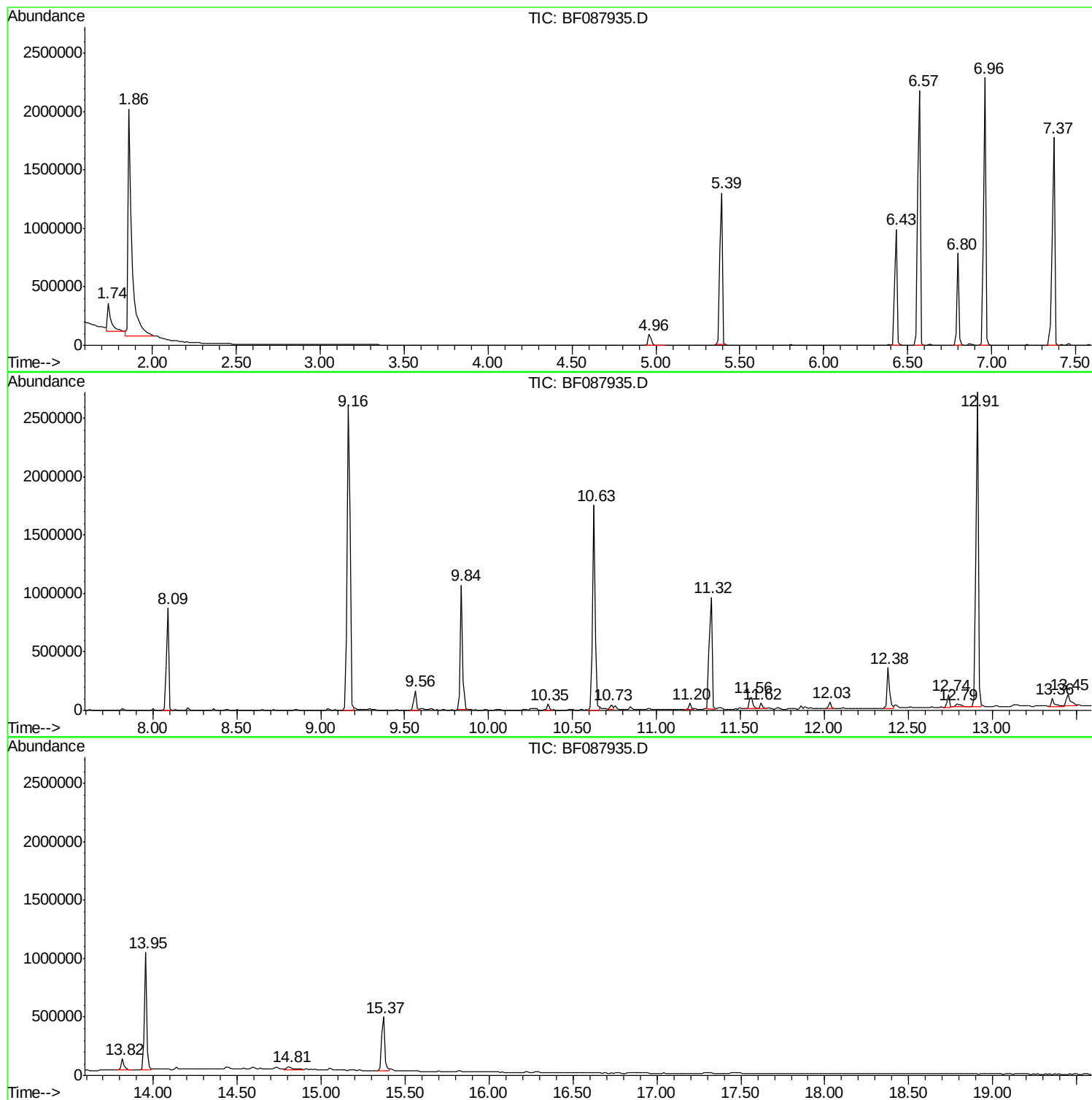
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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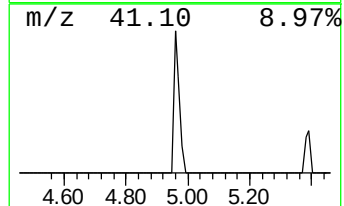
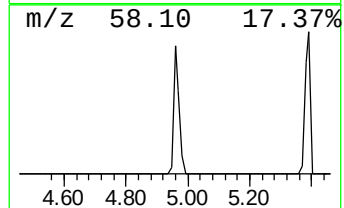
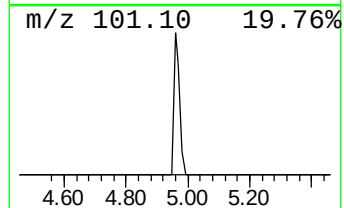
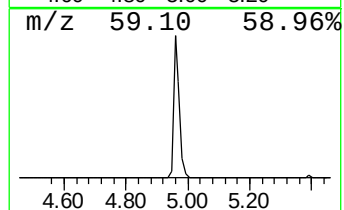
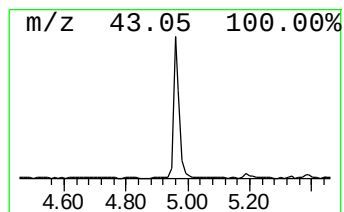
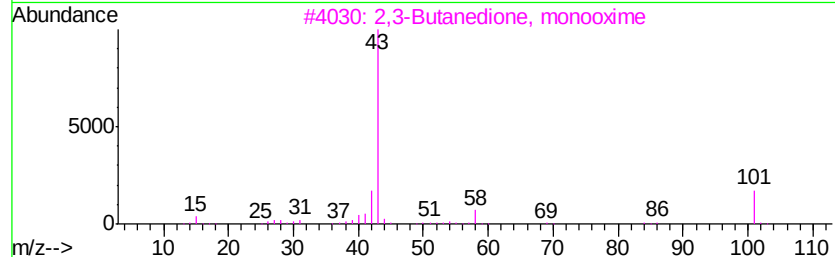
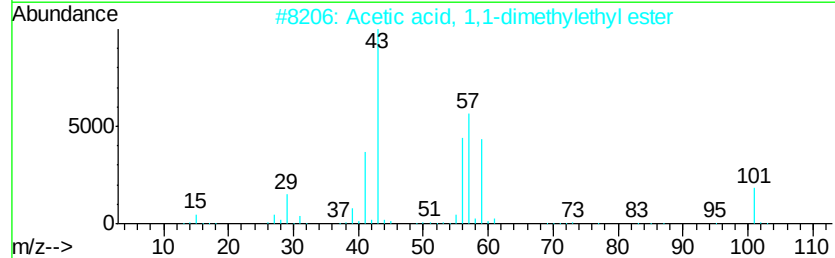
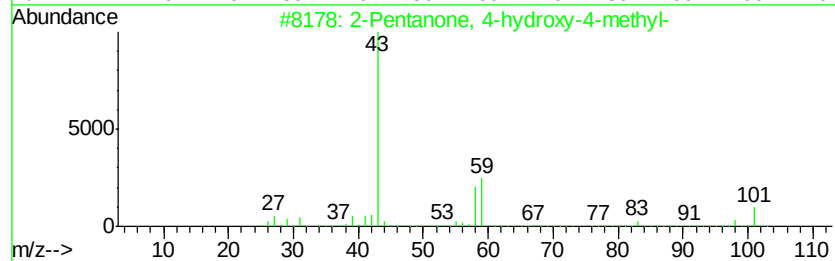
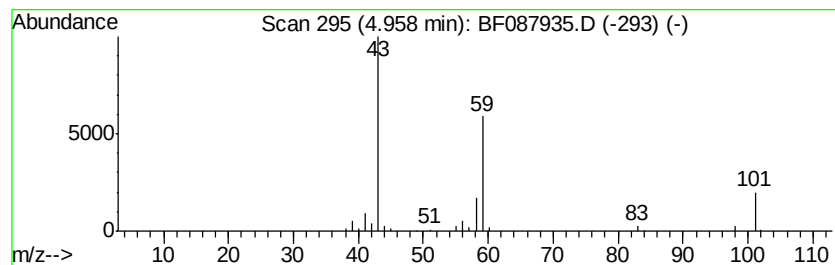
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	3.60 ng	116644	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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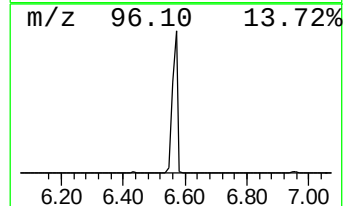
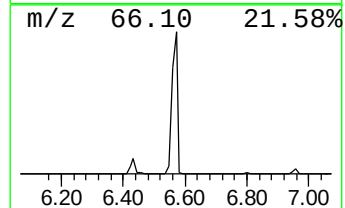
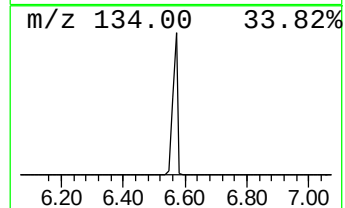
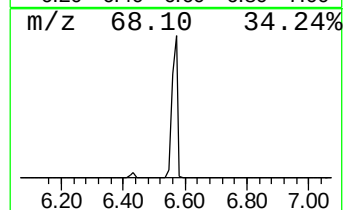
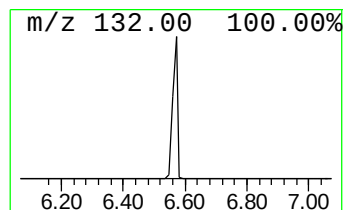
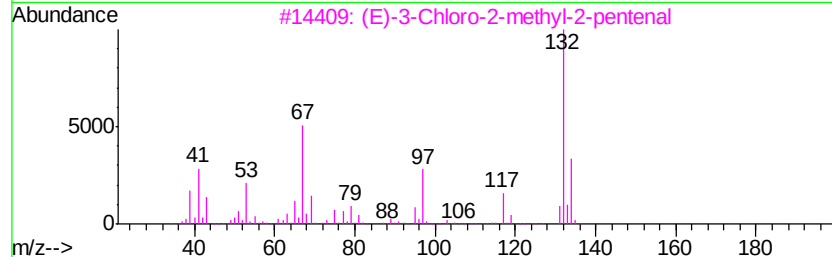
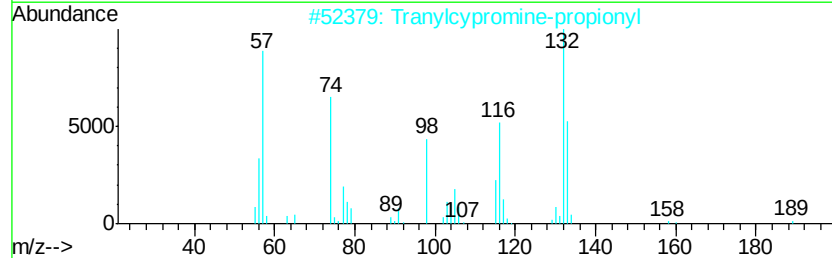
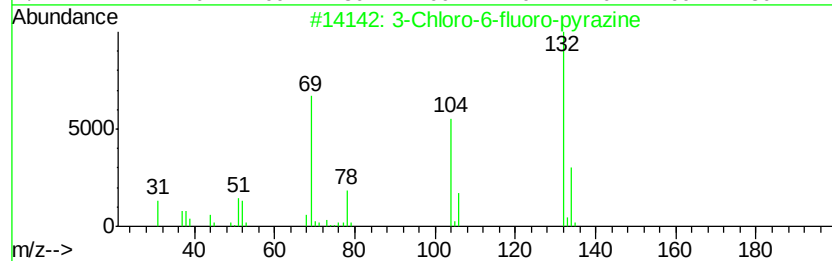
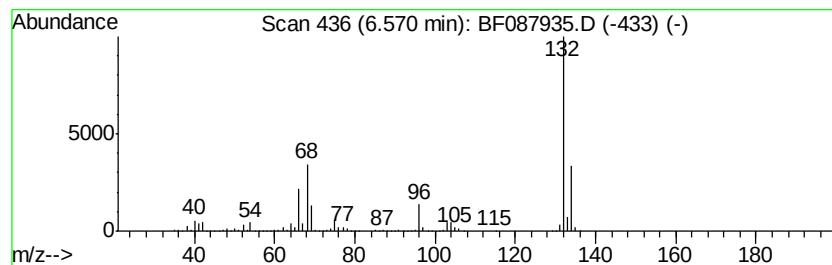
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Peak Number 4 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	78.43 ng	2542710	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		Xenon	132	Xe	007440-63-3	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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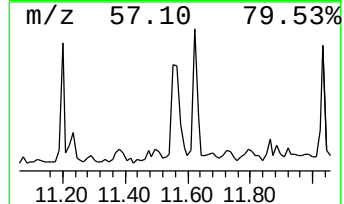
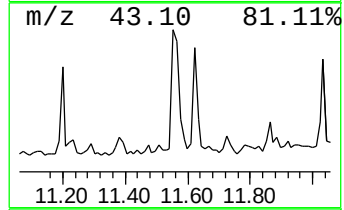
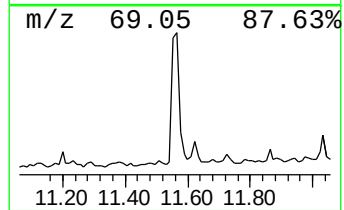
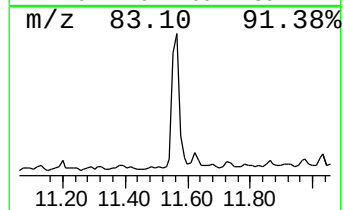
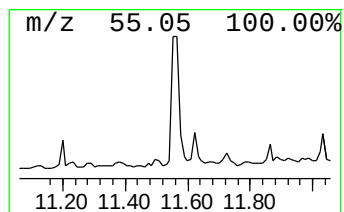
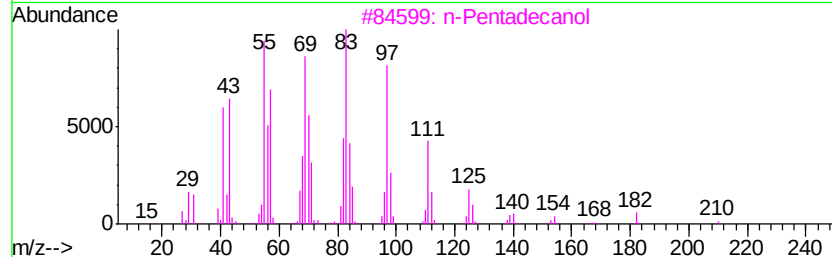
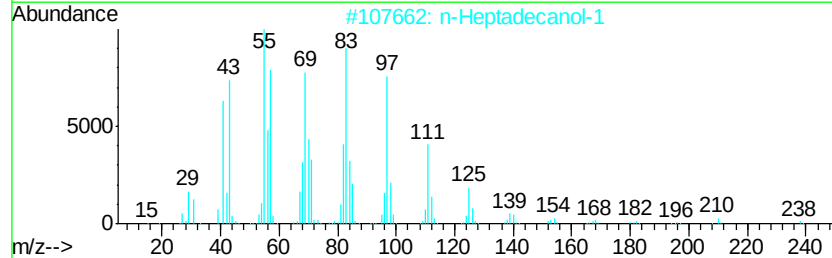
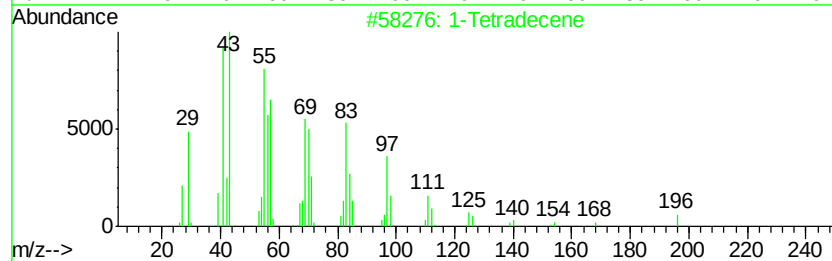
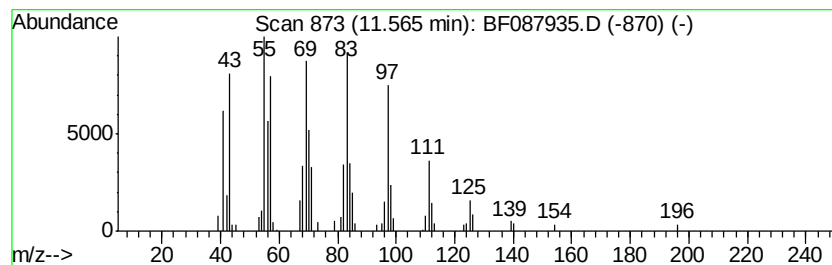
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Peak Number 6 1-Tetradecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.56	3.16 ng	158146	Phenanthrene-d10		11.32
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetradecene	196	C14H28	001120-36-1	96
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	95
3	n-Pentadecanol	228	C15H32O	000629-76-5	95
4	1-Hexadecanol	242	C16H34O	036653-82-4	95
5	1-Tetradecanol	214	C14H30O	000112-72-1	95



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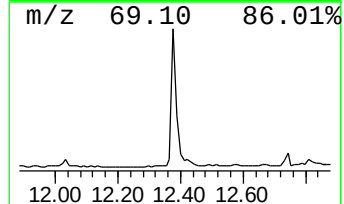
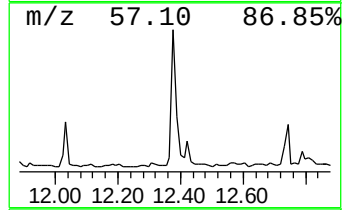
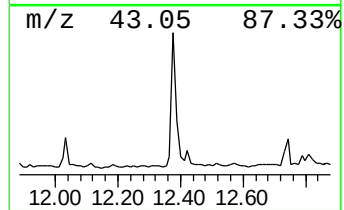
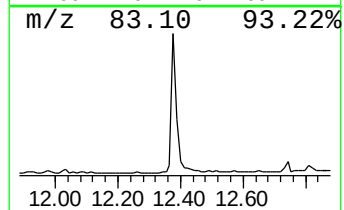
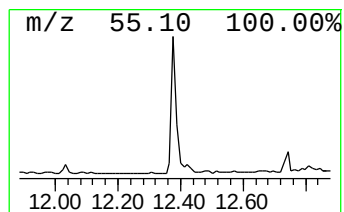
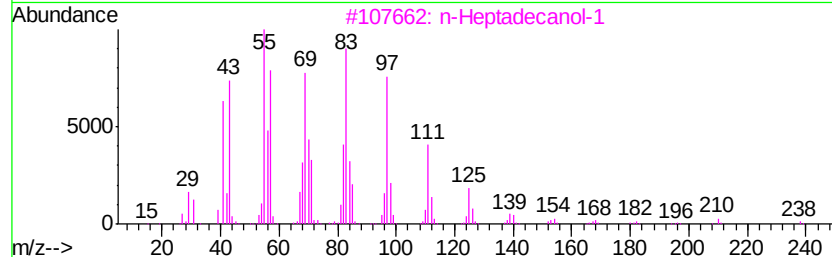
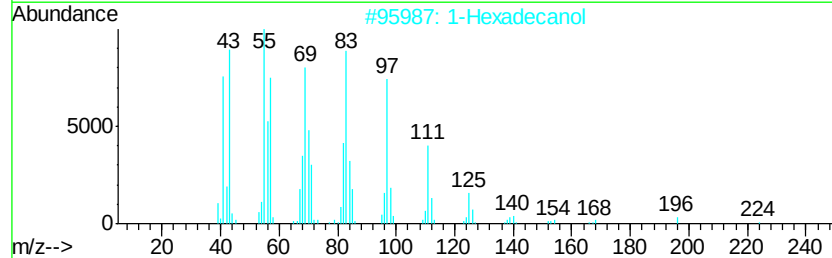
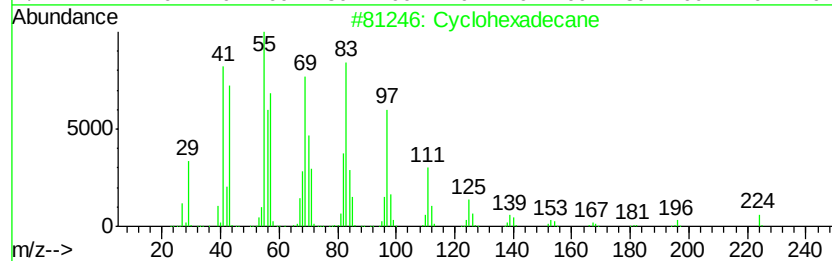
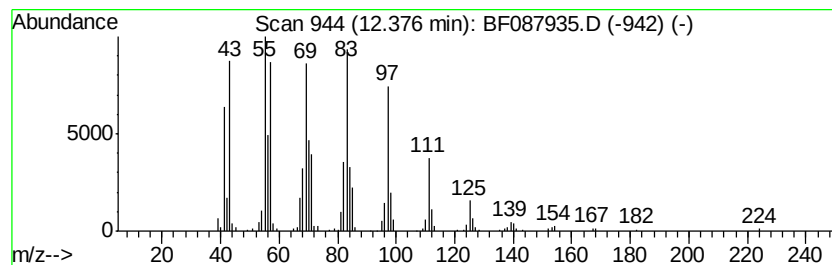
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Peak Number 7 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.38	7.54 ng	377704	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	98
2	1-Hexadecanol	242	C16H34O	036653-82-4	95
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	93



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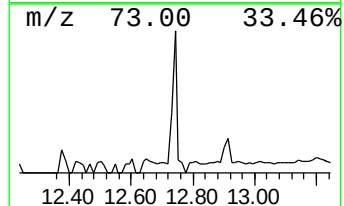
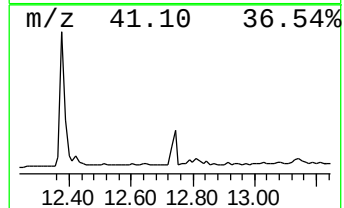
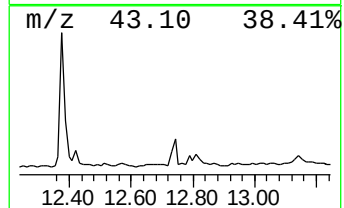
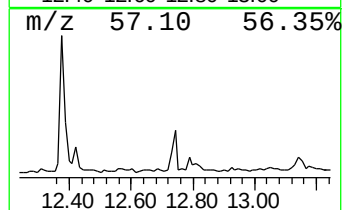
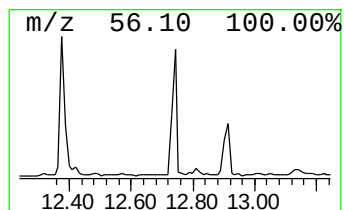
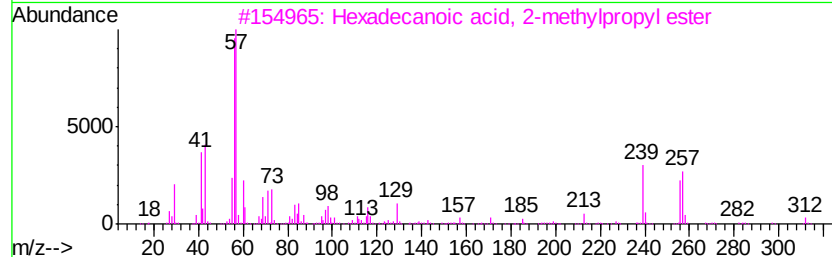
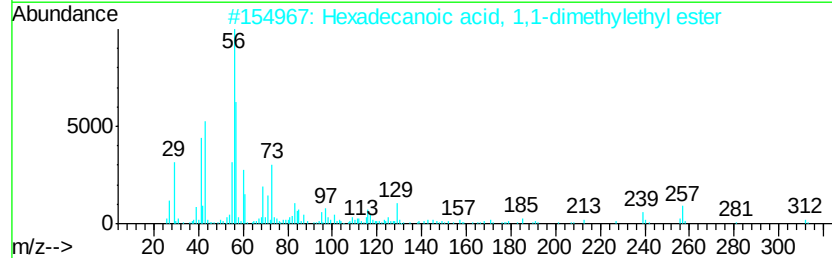
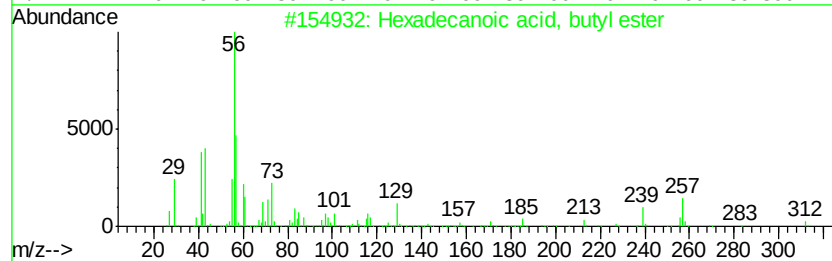
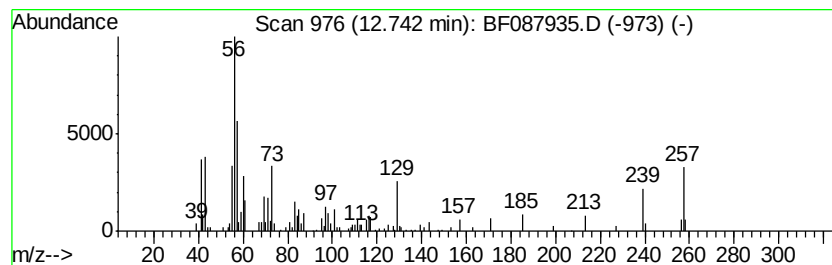
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Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	2.13 ng	103352	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	72
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	58
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	53
4		Nipecotic acid	129	C6H11NO2	000498-95-3	47
5		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	32



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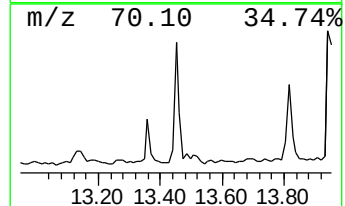
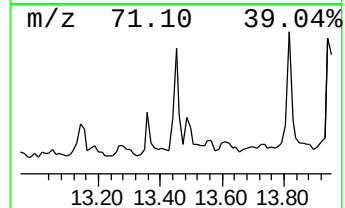
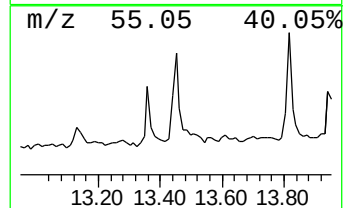
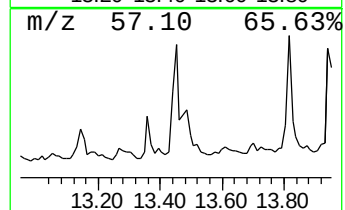
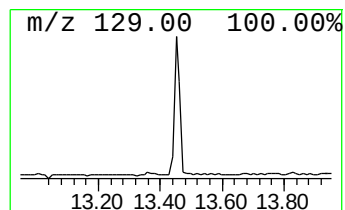
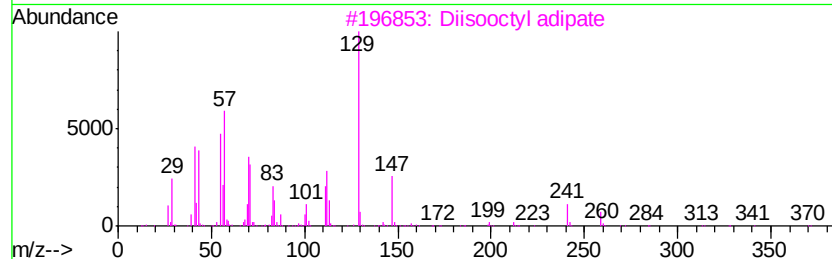
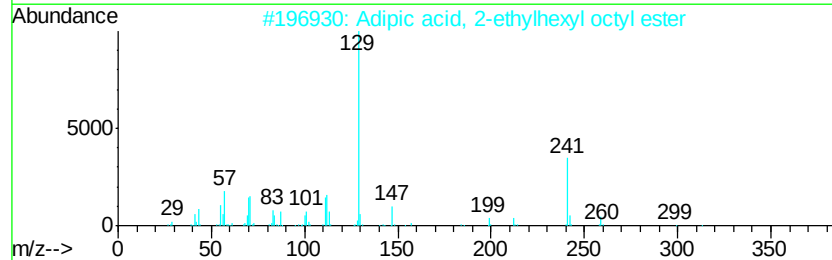
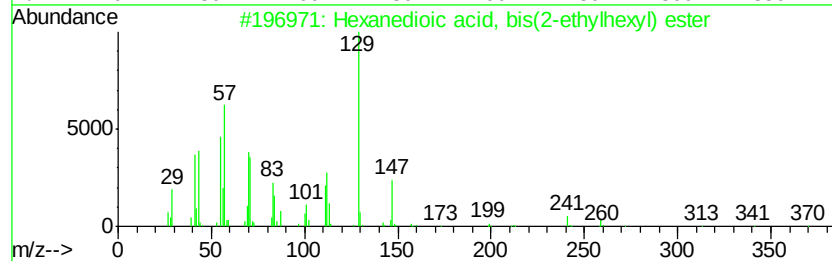
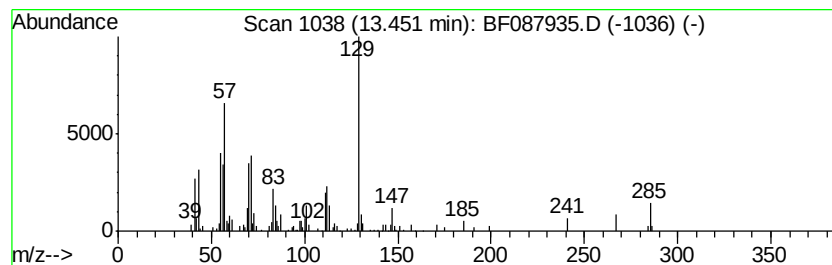
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexanedioic acid, bis(2-eth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	3.79 ng	183850	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	90
2		Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	90
3		Diisooctyl adipate	370	C22H42O4	001330-86-5	87
4		Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1000324-48-0	50
5		Adipic acid, cycloheptyl octyl e...	354	C21H38O4	1000324-72-1	47



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061116\
Data File : BF087935.D
Acq On : 12 Jun 2016 8:17
Operator : UM/SJ
Sample : H3504-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

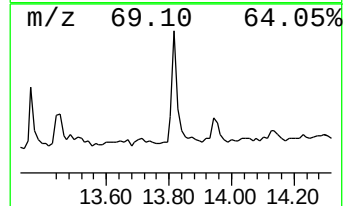
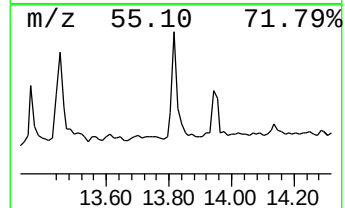
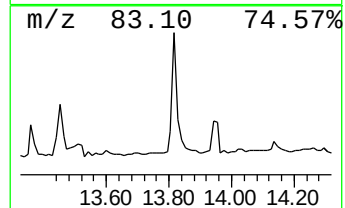
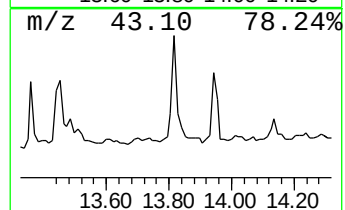
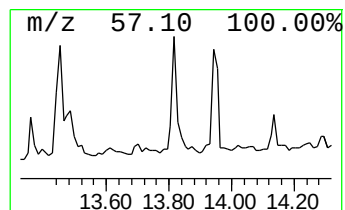
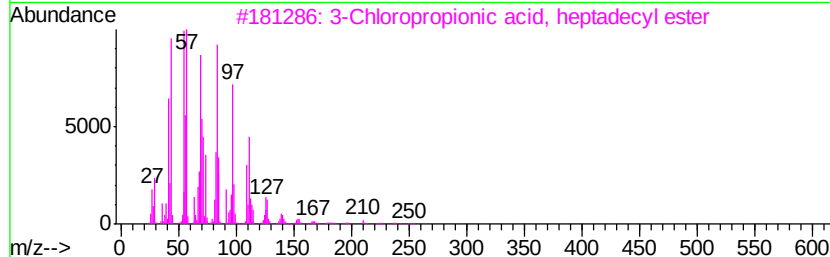
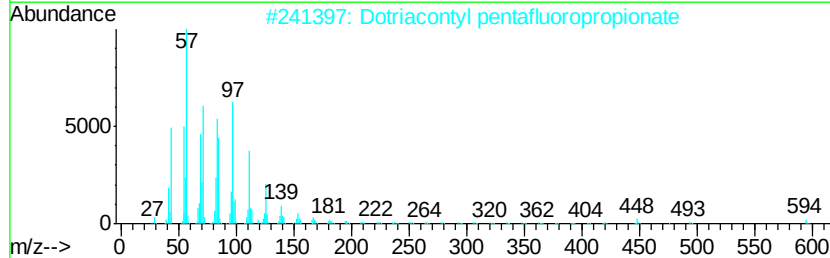
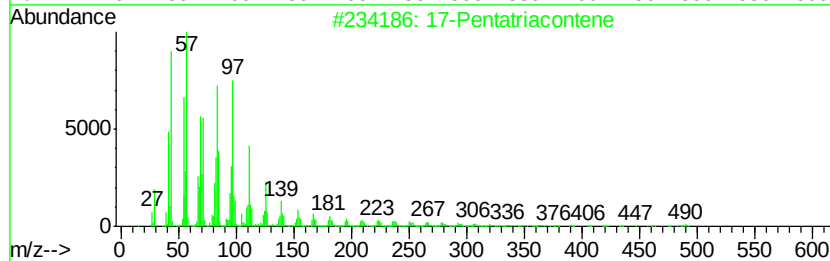
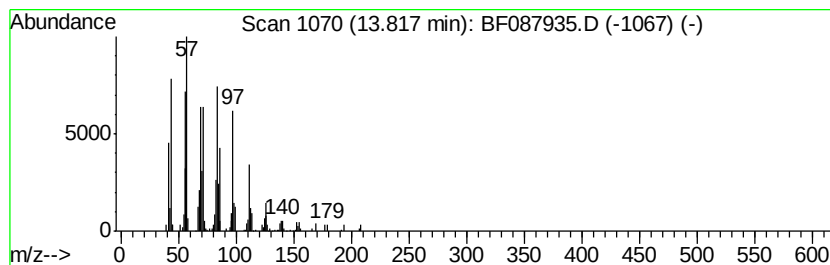
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 17-Pentatriacontene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	2.45 ng	118616	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	17-Pentatriacontene	491	C35H70	006971-40-0	91
2		Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	87
3		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	76
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	76
5		n-Heptadecanol-1	256	C17H36O	001454-85-9	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061116\
Data File : BF087935.D
Acq On : 12 Jun 2016 8:17
Operator : UM/SJ
Sample : H3504-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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...	4.96	3.6	ng	116644	1	6.80	648435	20.0
unknown6.57	6.57	78.4	ng	2542710	1	6.80	648435	20.0
1-Tetradecene	11.56	3.2	ng	158146	4	11.32	1001310	20.0
Cyclohexadecane	12.38	7.5	ng	377704	4	11.32	1001310	20.0
Hexadecanoic acid...	12.74	2.1	ng	103352	5	13.95	969080	20.0
Hexanedioic acid,...	13.45	3.8	ng	183850	5	13.95	969080	20.0
17-Pentatriacontene	13.82	2.5	ng	118616	5	13.95	969080	20.0