

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051216\
 Data File : BF086969.D
 Acq On : 13 May 2016 12:01
 Operator : UM/SJ
 Sample : H2916-03
 Misc :
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VITALE-FILL-CSPH3-3K

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-BF050916.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	1.633	3	4	12	rVB	585470	894222	13.74%	2.121%
2	1.747	12	14	51	rVB	2695720	6507246	100.00%	15.432%
3	4.764	276	278	292	rBV	357186	708656	10.89%	1.681%
4	5.222	315	318	320	rBV	2719644	3927215	60.35%	9.314%
5	6.285	408	411	414	rBV	3200912	3795086	58.32%	9.000%
6	6.399	418	421	423	rBV	3581872	4149726	63.77%	9.841%
7	6.616	438	440	443	rBV	756564	955762	14.69%	2.267%
8	6.776	452	454	457	rBV	3273370	2982386	45.83%	7.073%
9	7.199	488	491	493	rBV	2634065	2840935	43.66%	6.737%
10	7.908	551	553	556	rBV	1313379	1164452	17.89%	2.762%
11	8.993	645	648	650	rBV	3528128	3990547	61.32%	9.464%
12	9.382	680	682	685	rBV	269924	384547	5.91%	0.912%
13	9.599	699	701	703	rBV	116142	106650	1.64%	0.253%
14	9.656	703	706	708	rBV	1222308	1069142	16.43%	2.536%
15	10.102	742	745	746	rBV	191678	162622	2.50%	0.386%
16	10.319	761	764	767	rBV	67344	98789	1.52%	0.234%
17	10.445	772	775	777	rBV	1710566	1688571	25.95%	4.004%
18	10.571	784	786	793	rVB	212913	250035	3.84%	0.593%
19	11.016	823	825	826	rBV	102426	83884	1.29%	0.199%
20	11.131	833	835	838	rBV	887049	807390	12.41%	1.915%
21	12.719	971	974	976	rBV	2995471	2877759	44.22%	6.825%
22	13.634	1051	1054	1062	rBV	262998	680650	10.46%	1.614%
23	13.760	1062	1065	1070	rVV	920870	908759	13.97%	2.155%
24	13.851	1070	1073	1078	rVB2	35765	83457	1.28%	0.198%
25	15.120	1181	1184	1186	rBV	591362	668405	10.27%	1.585%
26	15.520	1217	1219	1223	rBV	42018	68817	1.06%	0.163%
27	15.634	1223	1229	1233	rVV3	29504	112315	1.73%	0.266%
28	15.943	1254	1256	1263	rVB3	25444	65426	1.01%	0.155%
29	16.183	1275	1277	1290	rVB2	43989	133390	2.05%	0.316%

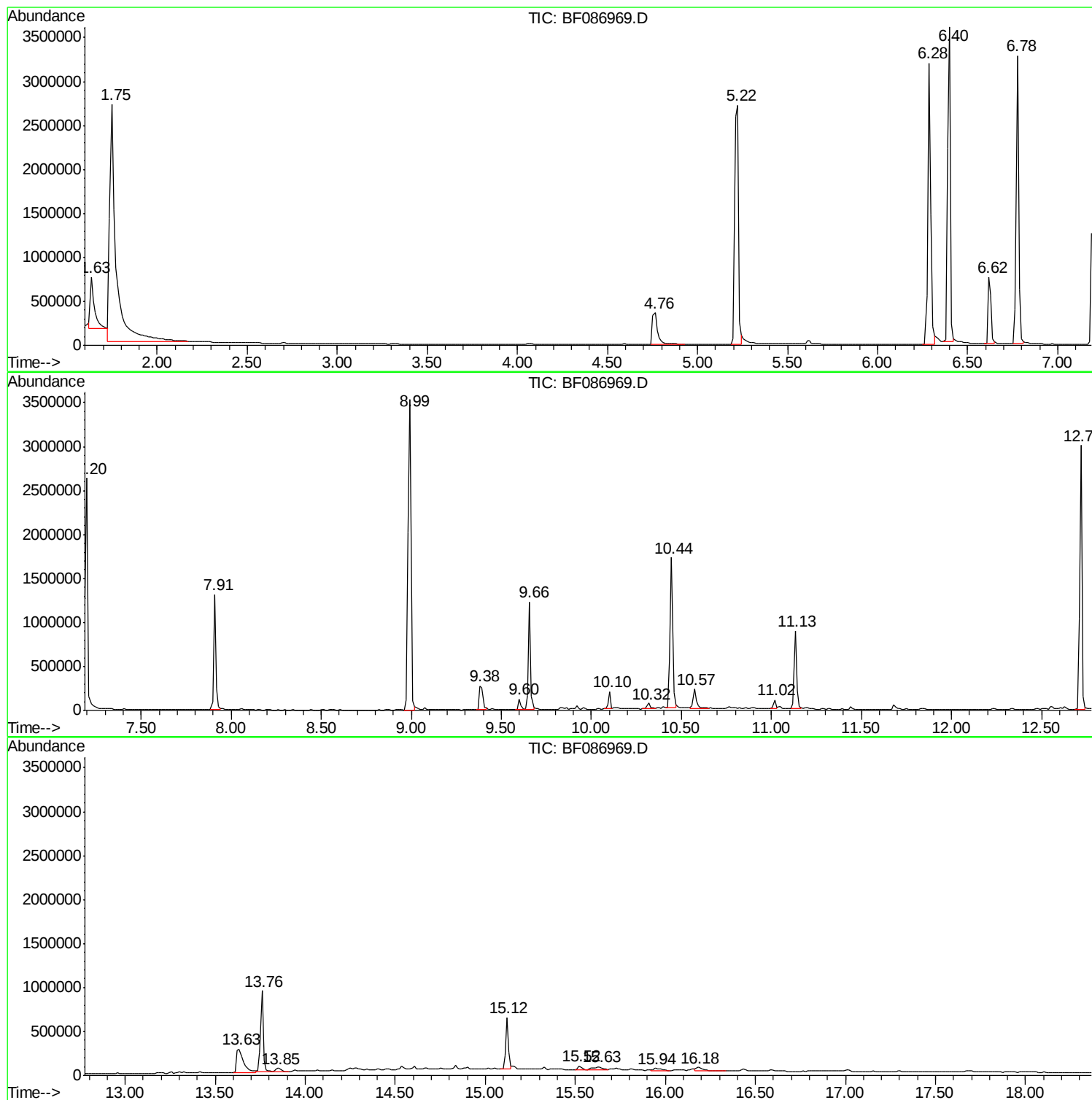
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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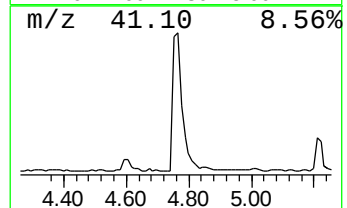
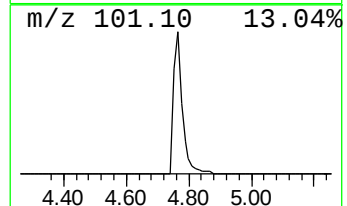
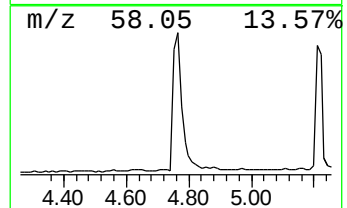
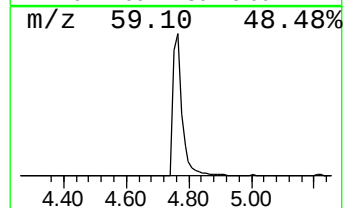
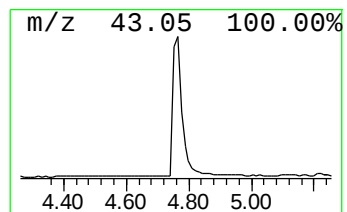
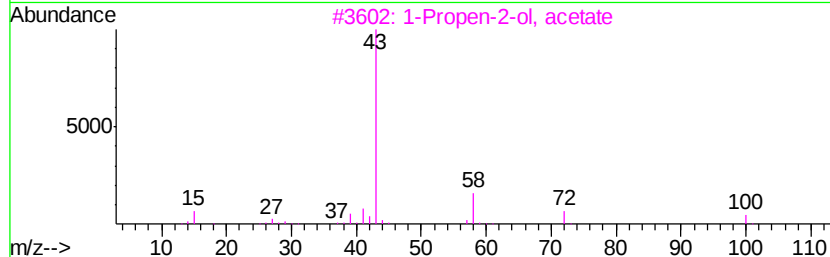
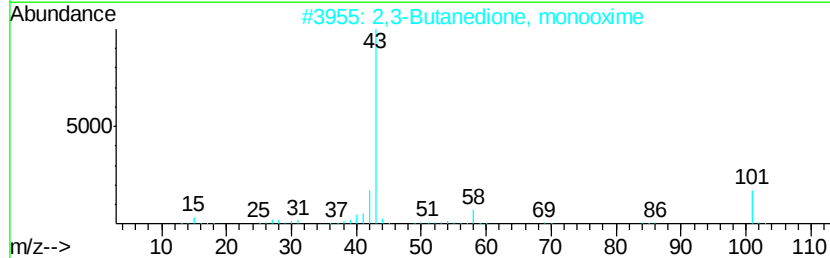
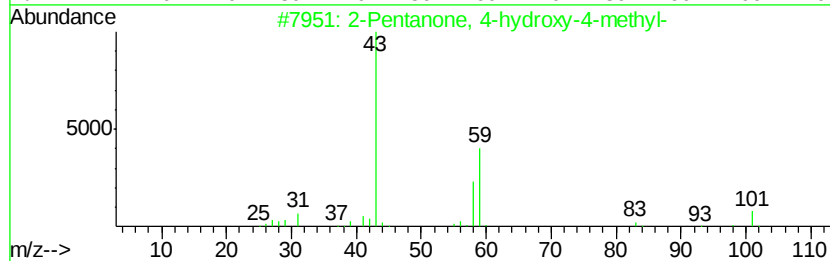
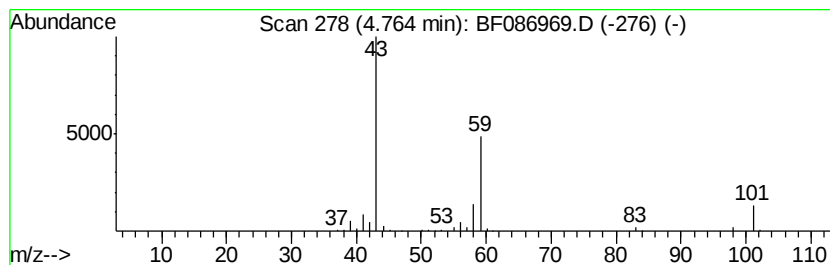
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	14.83 ng	708656	1,4-Dichlorobenzene-d4	6.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Acetic acid, 2-propenyl ester	100	C5H8O2	000591-87-7	9
5		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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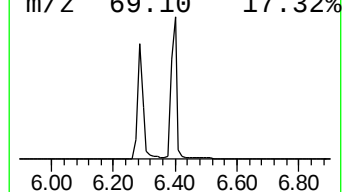
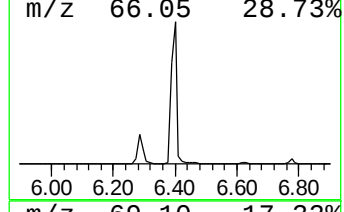
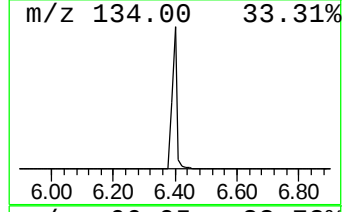
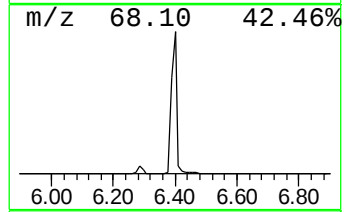
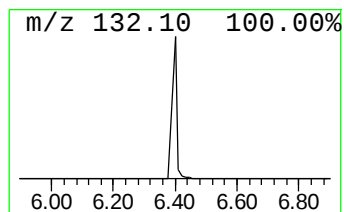
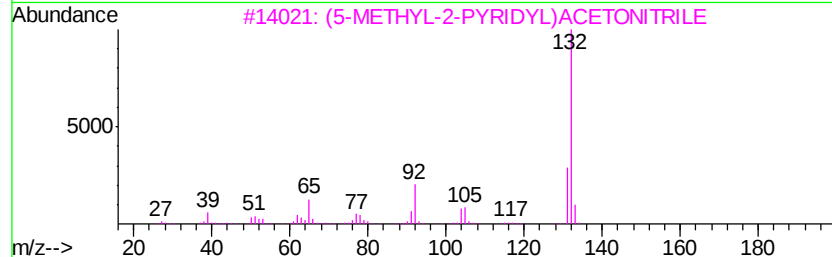
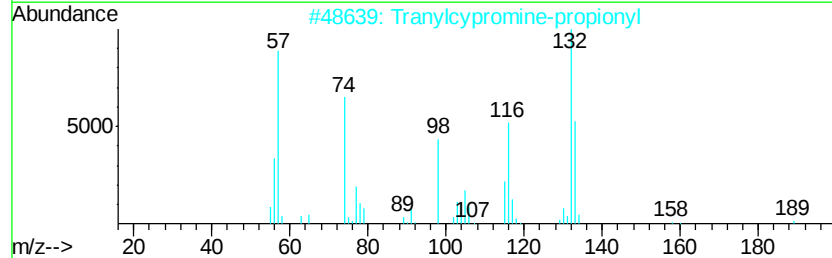
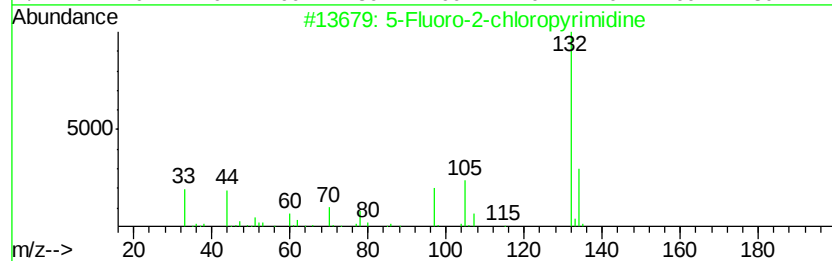
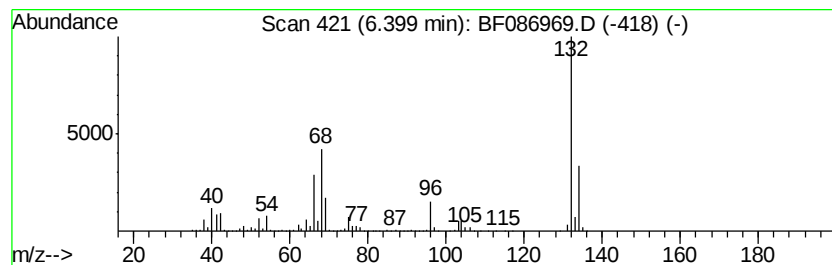
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Peak Number 4 unknown6.40 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	86.84 ng	4149730	1,4-Dichlorobenzene-d4	6.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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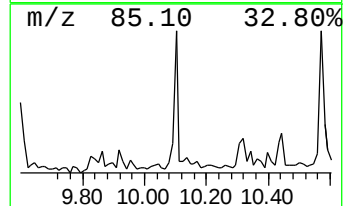
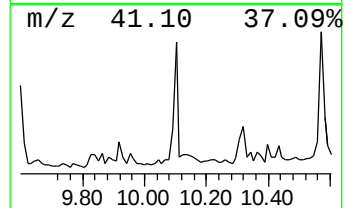
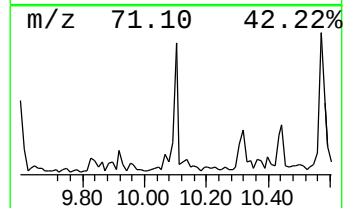
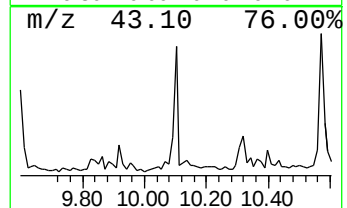
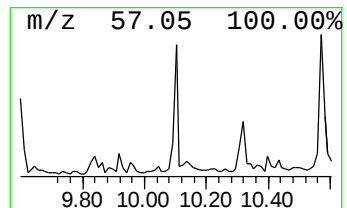
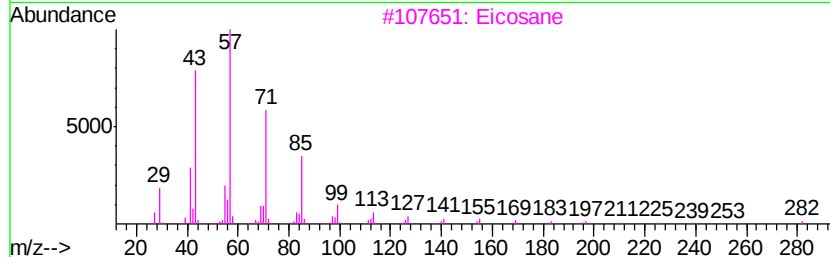
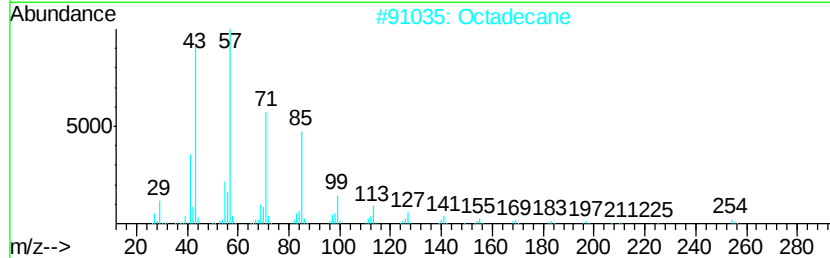
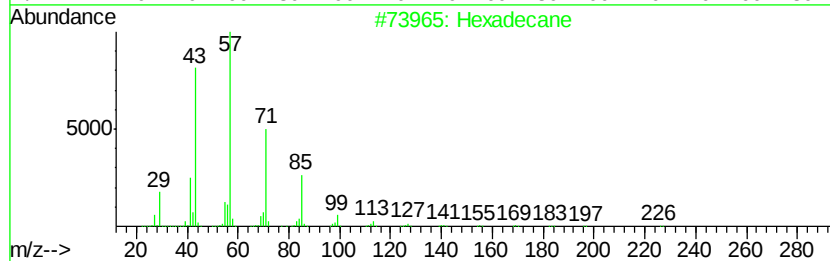
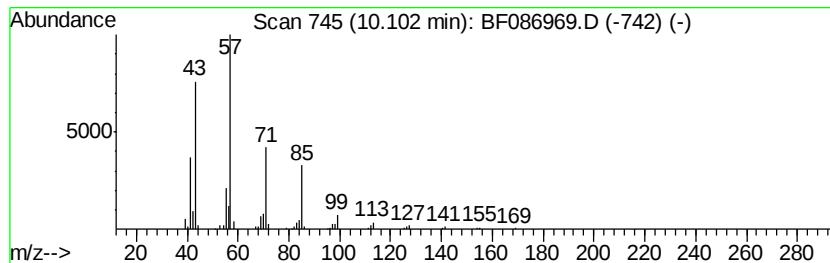
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.10	3.04 ng	162622	Acenaphthene-d10	9.66	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Octadecane	254	C18H38	000593-45-3	86
3	Eicosane	282	C20H42	000112-95-8	86
4	Tridecane	184	C13H28	000629-50-5	83
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	78



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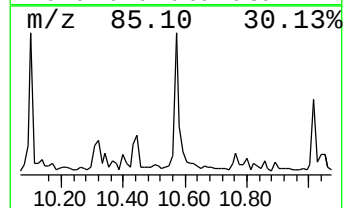
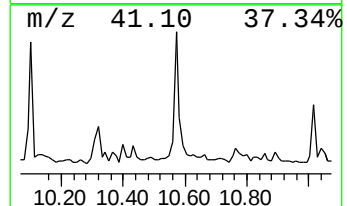
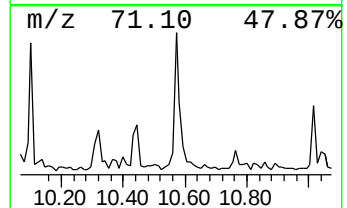
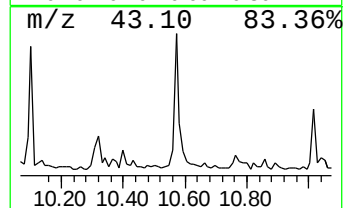
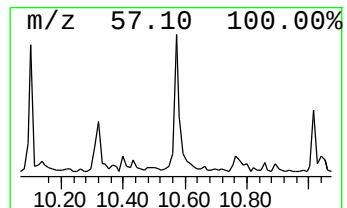
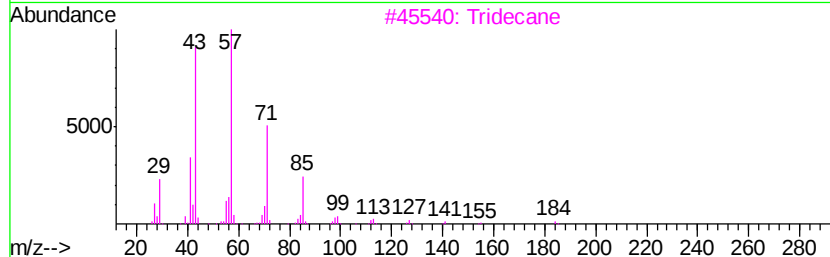
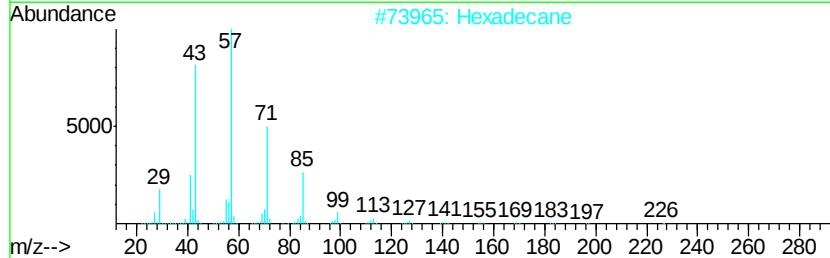
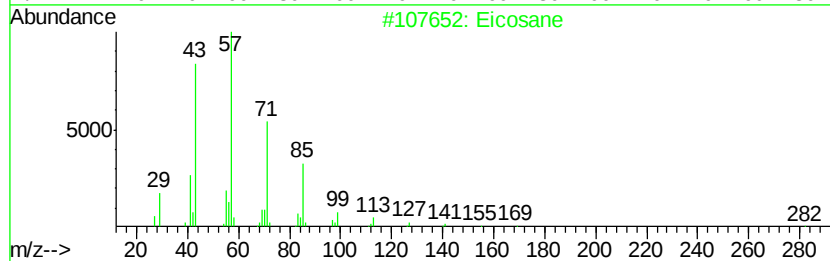
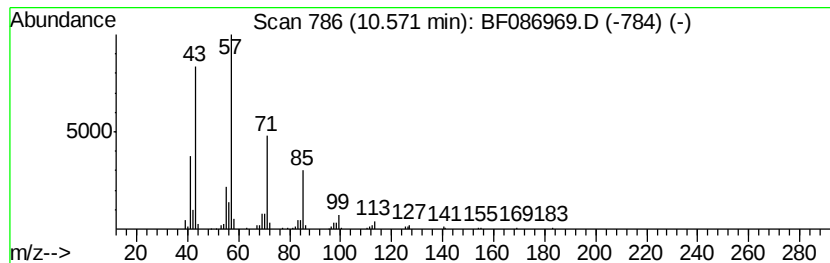
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Peak Number 7 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.57	6.19 ng	250035	Phenanthrene-d10	11.13	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	91
3	Tridecane	184	C13H28	000629-50-5	90
4	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	90
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86



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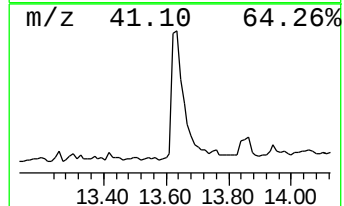
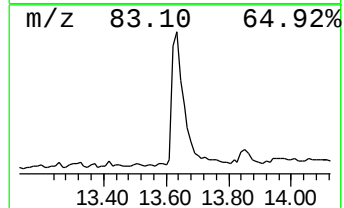
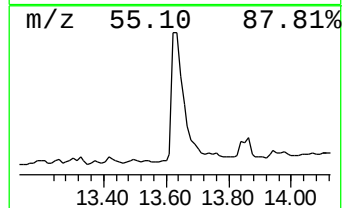
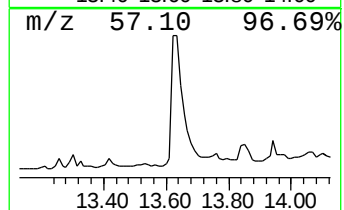
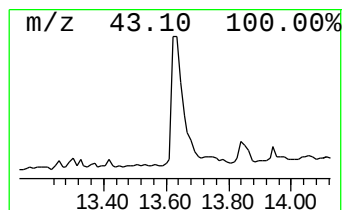
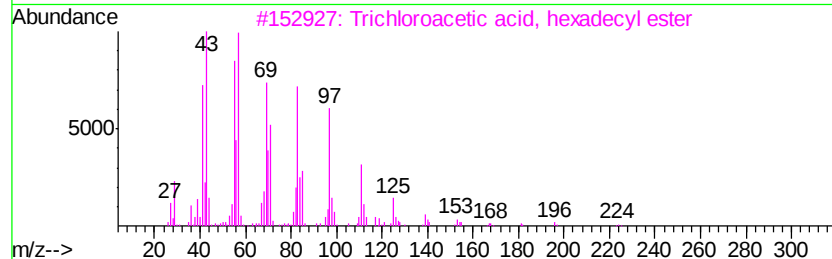
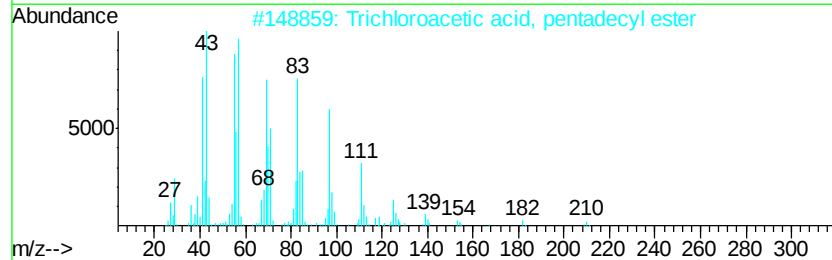
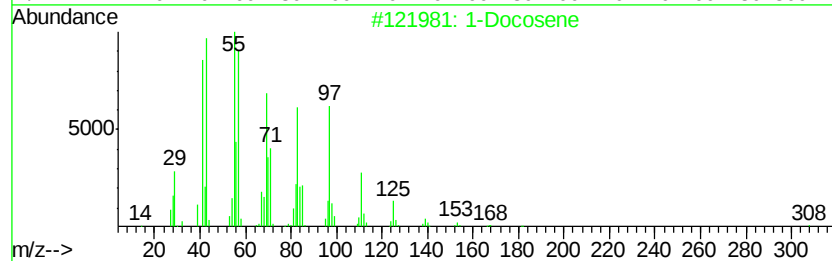
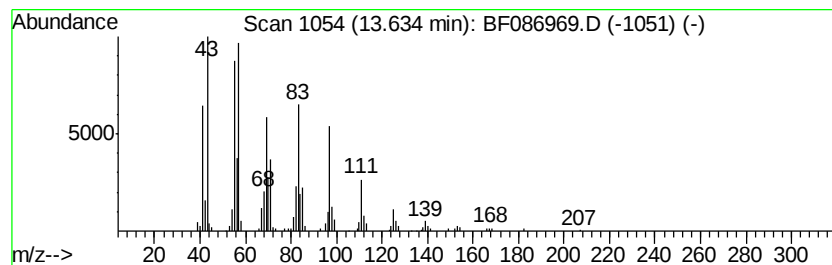
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Peak Number 9 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	14.98 ng	680650	Chrysene-d12	13.76
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Docosene		308 C22H44	001599-67-3 95
2	Trichloroacetic acid, pentadecyl...		372 C17H31Cl3O2	074339-53-0 95
3	Trichloroacetic acid, hexadecyl ...		386 C18H33Cl3O2	074339-54-1 93
4	1-Nonadecene		266 C19H38	018435-45-5 90
5	Trichloroacetic acid, tetradecyl...		358 C16H29Cl3O2	074339-52-9 87



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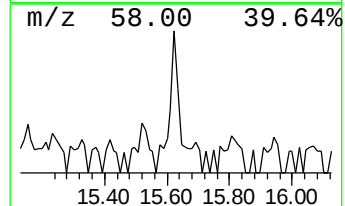
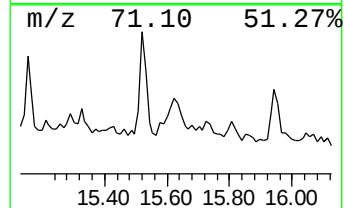
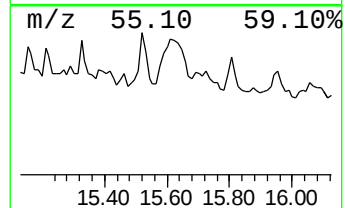
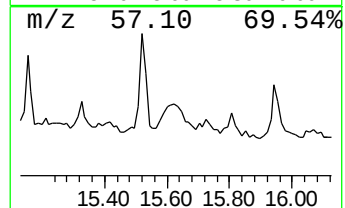
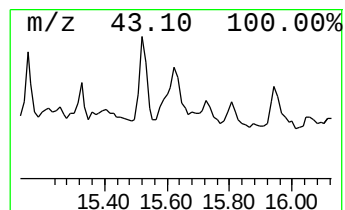
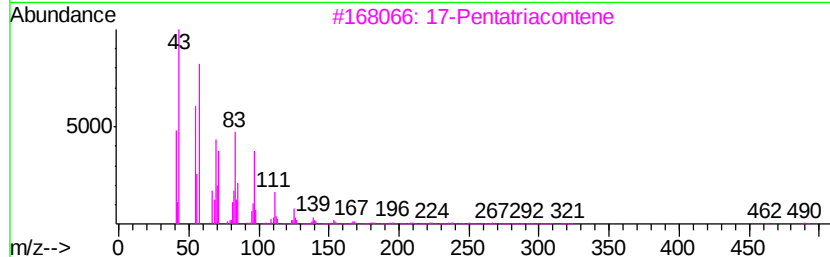
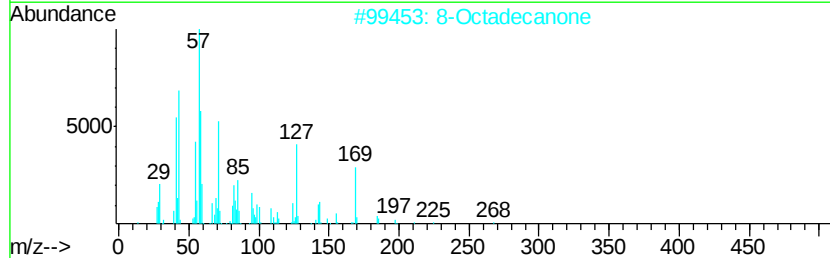
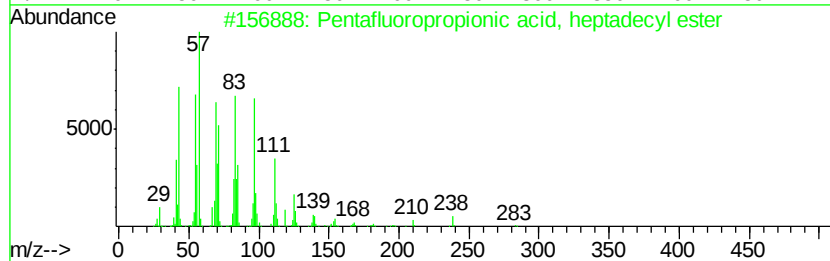
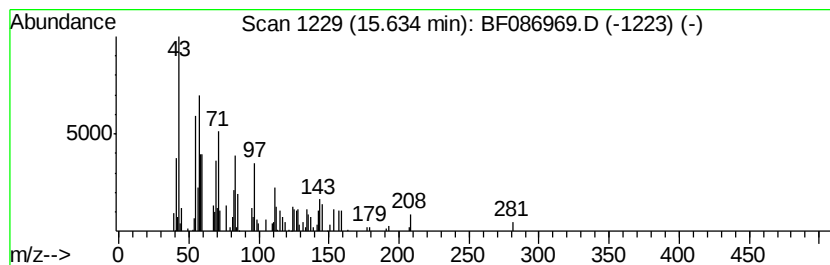
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown15.63 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.63	3.36 ng	112315	Perylene-d12	15.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	27
2		8-Octadecanone	268	C18H36O	079246-41-6	27
3		17-Pentatriacontene	491	C35H70	006971-40-0	27
4		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	27
5		1-Tridecene	182	C13H26	002437-56-1	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051216\
Data File : BF086969.D
Acq On : 13 May 2016 12:01
Operator : UM/SJ
Sample : H2916-03
Misc :
ALS Vial : 43 Sample Multiplier: 1

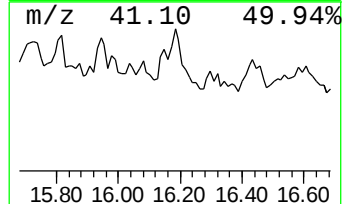
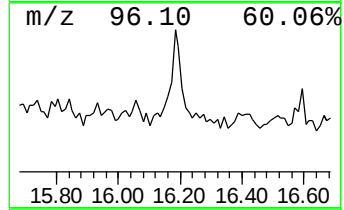
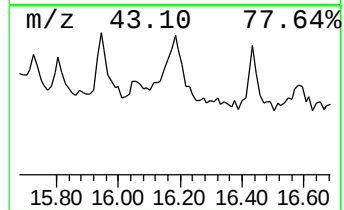
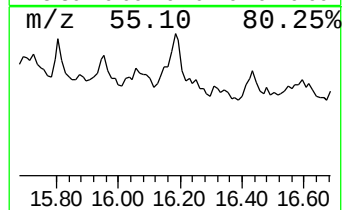
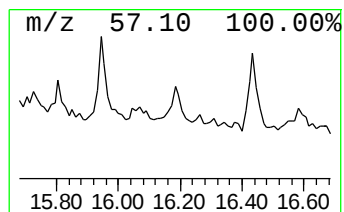
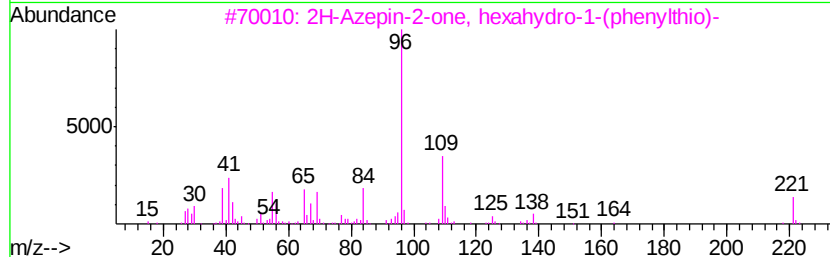
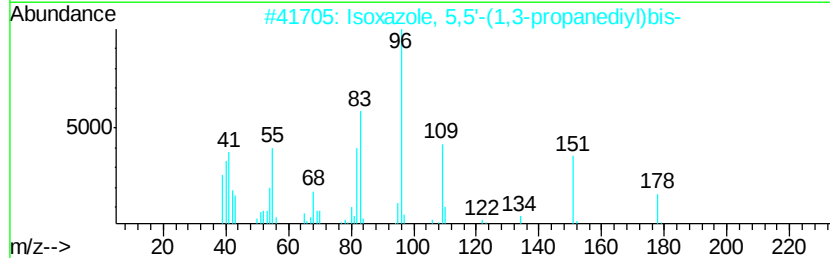
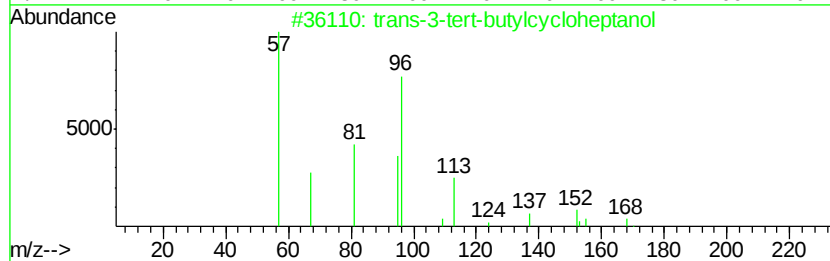
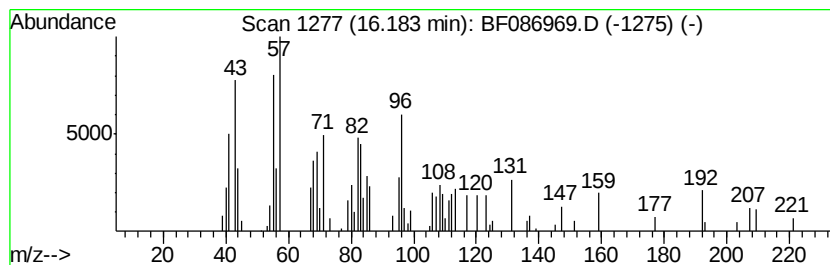
Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-3K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown16.18 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	3.99 ng	133390	Perylene-d12	15.12
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	trans-3-tert-butylcycloheptanol	170 C11H22O	019790-14-8	22
2	Isoxazole, 5,5'-(1,3-propanediyl...	178 C9H10N2O2	037704-51-1	14
3	2H-Azepin-2-one, hexahydro-1-(ph...	221 C12H15NOS	036452-23-0	14
4	1H-Imidazole-4-ethanamine, 2-met...	125 C6H11N3	034392-54-6	14
5	(E)-2-Decenyl acetate	198 C12H22O2	002497-23-6	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051216\
Data File : BF086969.D
Acq On : 13 May 2016 12:01
Operator : UM/SJ
Sample : H2916-03
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-3K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.76	14.8	ng	708656	1	6.62	955762	20.0
unknown6.40	6.40	86.8	ng	4149730	1	6.62	955762	20.0
Hexadecane	10.10	3.0	ng	162622	3	9.66	1069140	20.0
Eicosane	10.57	6.2	ng	250035	4	11.13	807390	20.0
1-Docosene	13.63	15.0	ng	680650	5	13.76	908759	20.0
unknown15.63	15.63	3.4	ng	112315	6	15.12	668405	20.0
unknown16.18	16.18	4.0	ng	133390	6	15.12	668405	20.0