

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100516\
 Data File : BF090397.D
 Acq On : 5 Oct 2016 23:18
 Operator : UM/SJ
 Sample : H5061-19
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SUP-B003-25-30

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-BF100516.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	3.468	97	99	114	rBV	75848	203252	2.64%	0.300%
2	5.206	248	251	258	rVB	1146992	1669580	21.70%	2.467%
3	5.617	283	287	289	rBV	6228655	7692326	100.00%	11.365%
4	6.623	372	375	378	rBV	5939514	6544957	85.08%	9.670%
5	6.771	385	388	390	rBV	7066244	7407828	96.30%	10.945%
6	7.000	406	408	410	rBV	2136417	1719218	22.35%	2.540%
7	7.160	419	422	424	rVB	5737333	5102894	66.34%	7.539%
8	7.560	454	457	460	rBV	3790940	4122382	53.59%	6.091%
9	7.640	460	464	469	rVB	78958	119641	1.56%	0.177%
10	8.292	518	521	523	rBV	2517402	2394249	31.13%	3.537%
11	9.366	612	615	618	rBV	6141830	6868594	89.29%	10.148%
12	9.766	647	650	652	rBV	2041192	2267590	29.48%	3.350%
13	9.903	660	662	665	rVB	127181	135721	1.76%	0.201%
14	10.052	672	675	677	rVB	3148309	2737918	35.59%	4.045%
15	10.486	709	713	714	rBV	106871	141417	1.84%	0.209%
16	10.840	741	744	746	rBV	4664681	4507719	58.60%	6.660%
17	10.955	752	754	759	rVB	157721	188887	2.46%	0.279%
18	11.412	791	794	795	rBV	74576	105797	1.38%	0.156%
19	11.538	803	805	808	rBV	2509941	2263816	29.43%	3.345%
20	12.063	849	851	860	rBV	501208	535697	6.96%	0.791%
21	12.669	902	904	909	rVB	61927	81548	1.06%	0.120%
22	12.772	909	913	918	rBV4	39582	112499	1.46%	0.166%
23	12.852	918	920	927	rBV	286013	324484	4.22%	0.479%
24	13.138	942	945	947	rBV	6428057	6940151	90.22%	10.254%
25	14.052	1022	1025	1031	rBV	205359	404374	5.26%	0.597%
26	14.189	1034	1037	1039	rBV	1977287	1810408	23.54%	2.675%
27	15.698	1165	1169	1171	rBV	839938	1279207	16.63%	1.890%

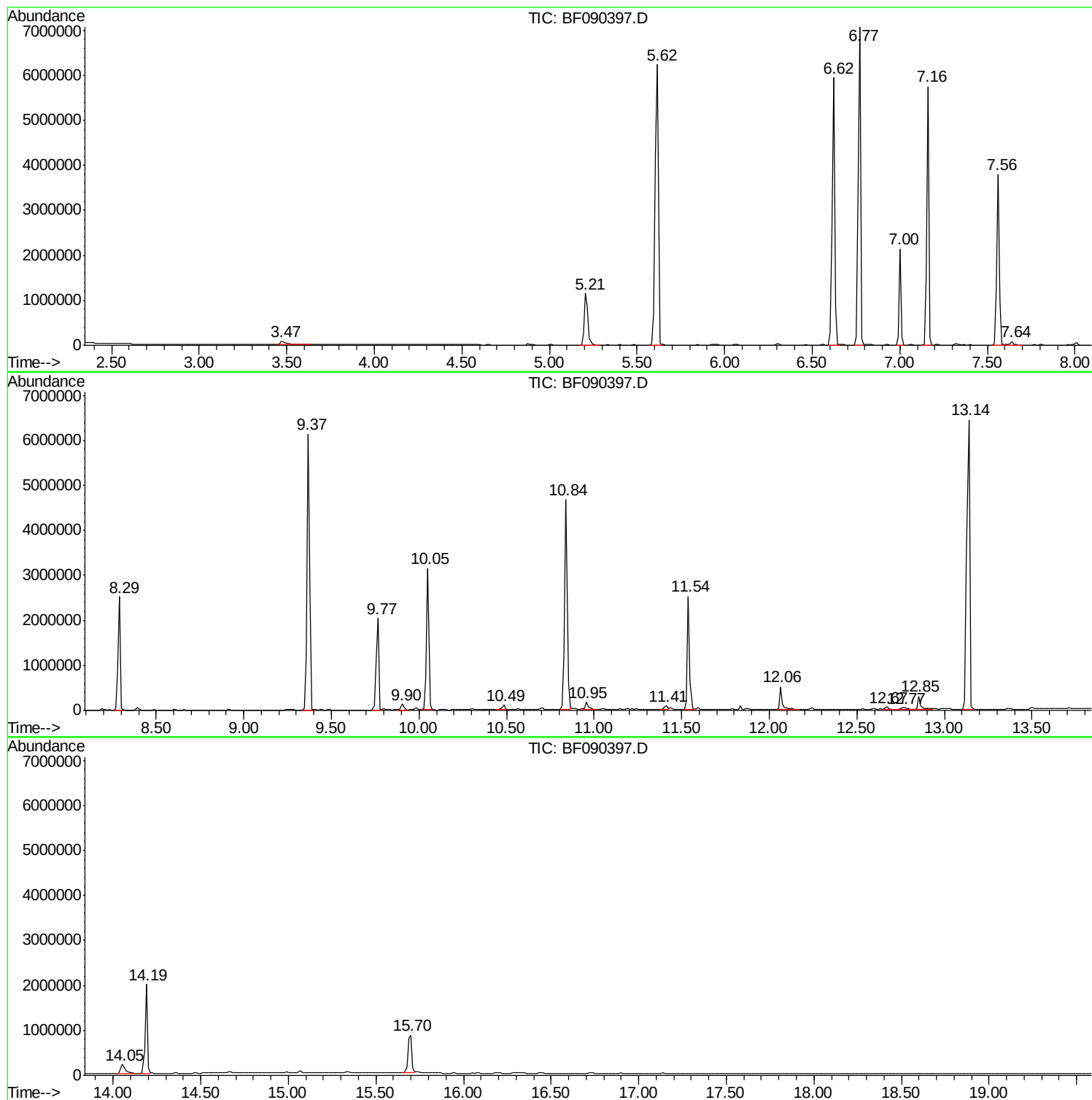
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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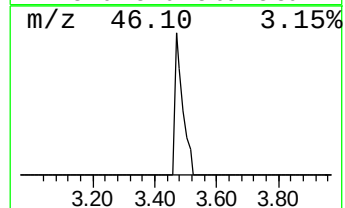
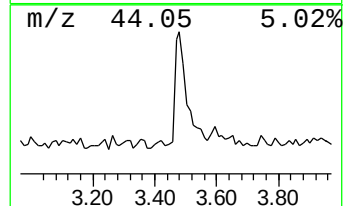
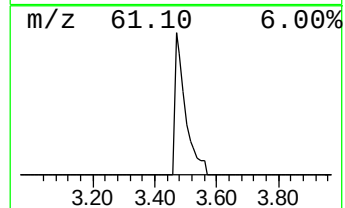
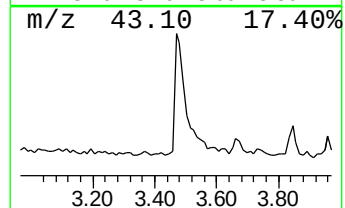
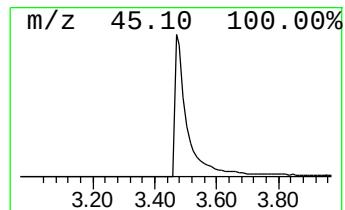
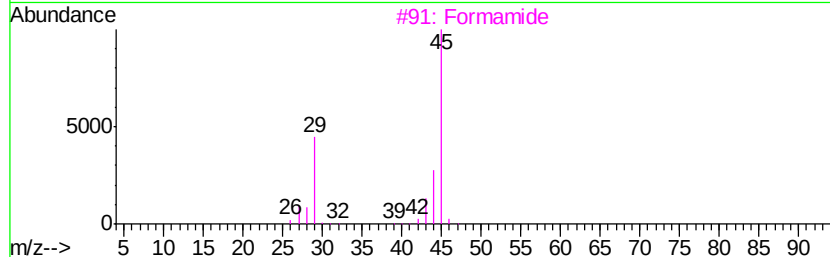
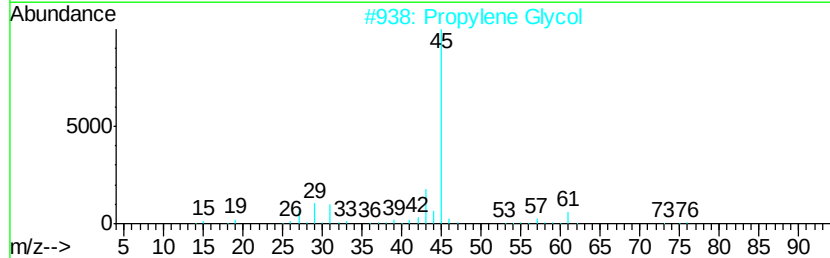
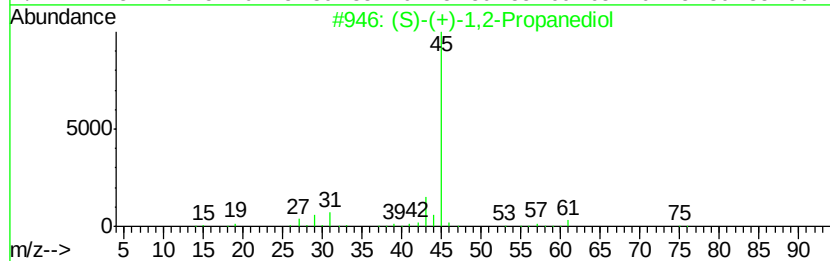
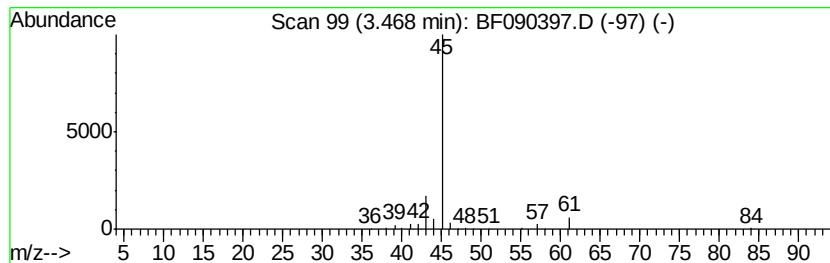
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.47 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.47	2.36 ng	203252	1,4-Dichlorobenzene-d4	7.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43	
2	Propylene Glycol	76	C3H8O2	000057-55-6	9	
3	Formamide	45	CH3NO	000075-12-7	7	
4	L-Lactic acid	90	C3H6O3	000079-33-4	4	
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	4	



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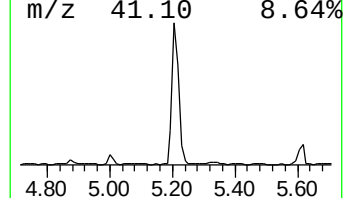
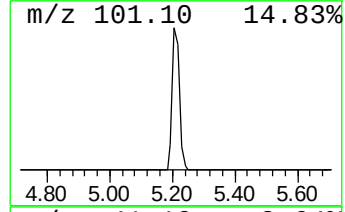
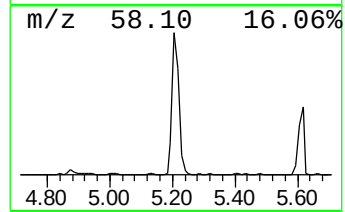
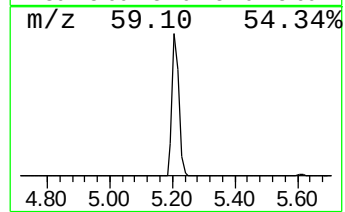
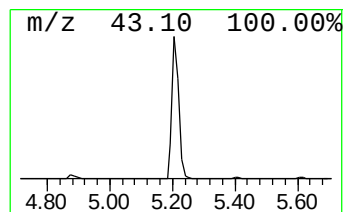
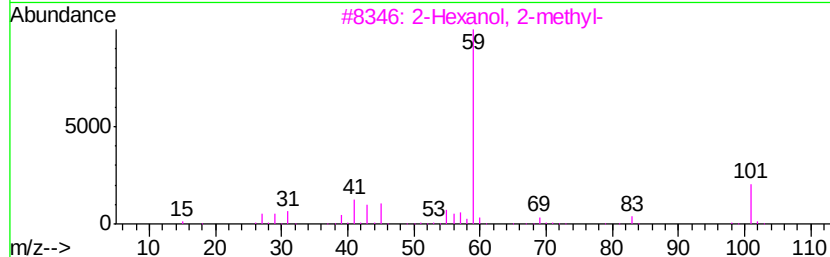
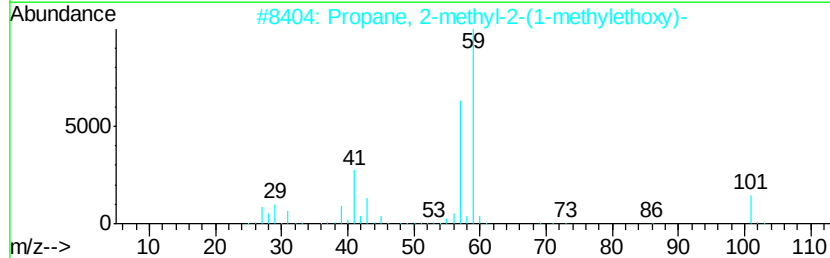
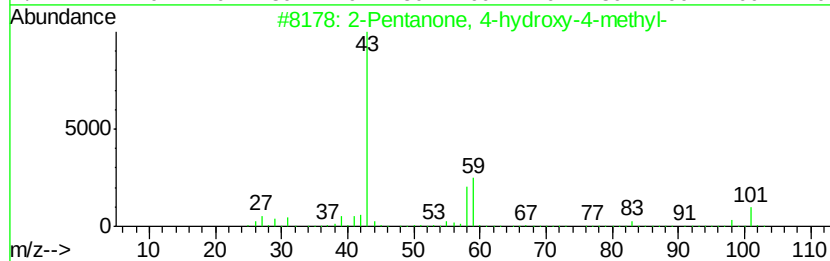
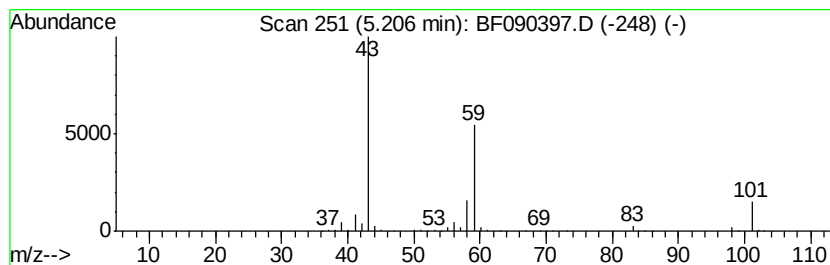
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	19.42 ng	1669580	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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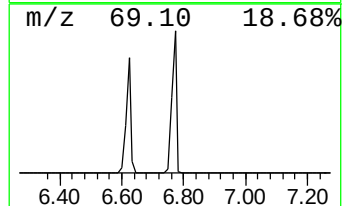
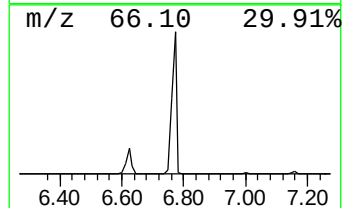
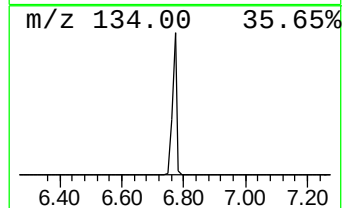
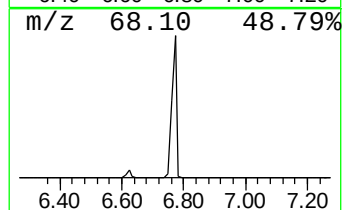
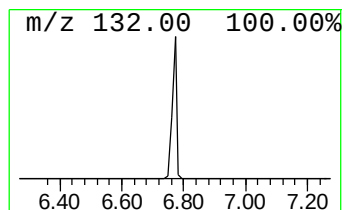
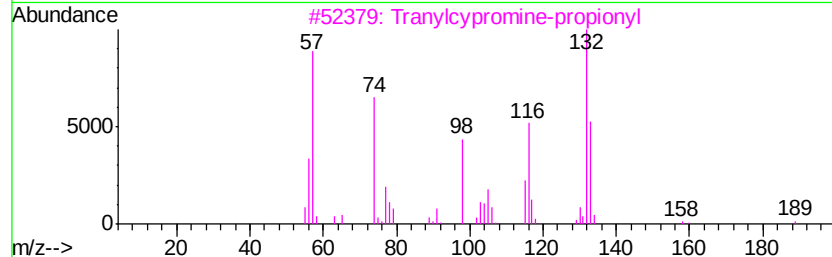
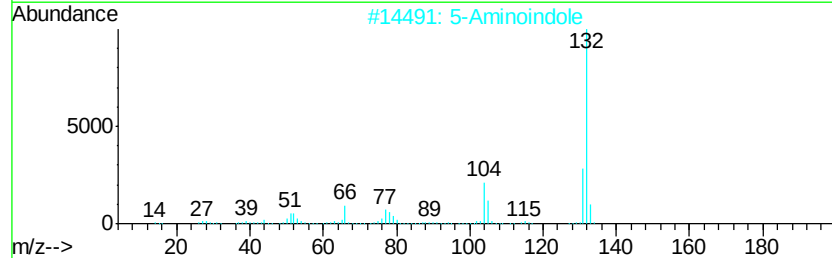
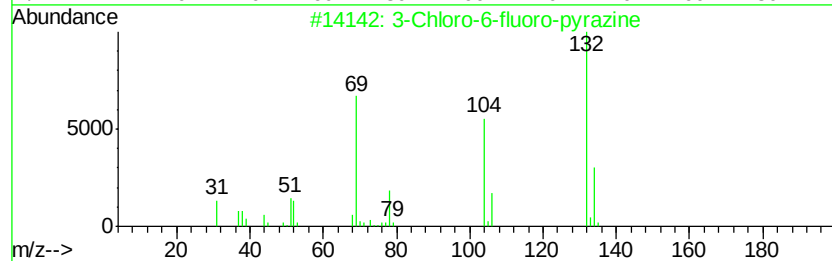
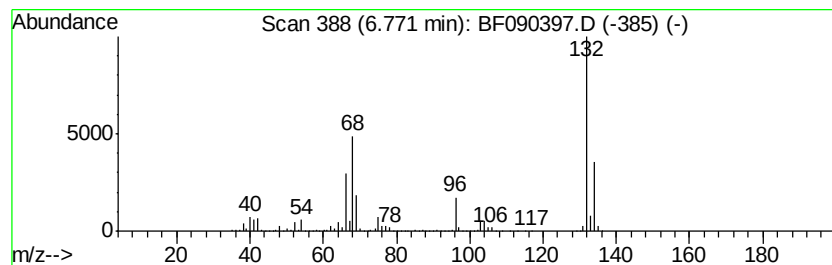
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Peak Number 3 unknown6.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	86.18 ng	7407830	1,4-Dichlorobenzene-d4	7.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3		Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5		Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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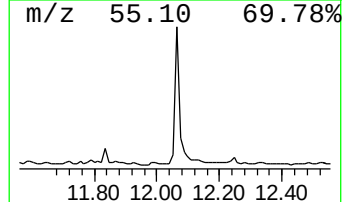
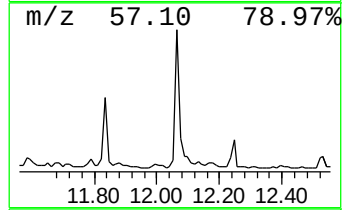
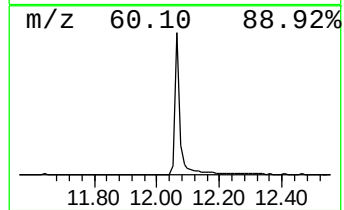
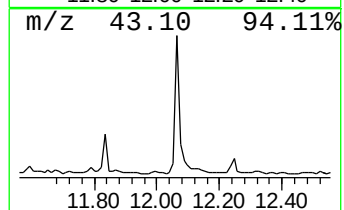
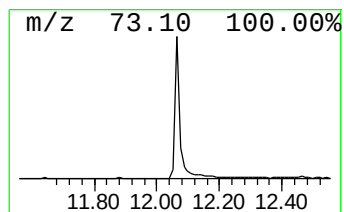
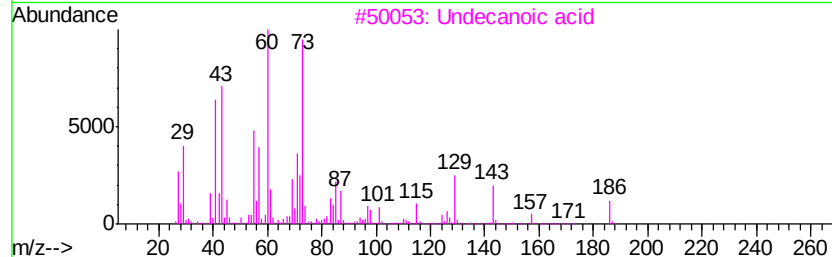
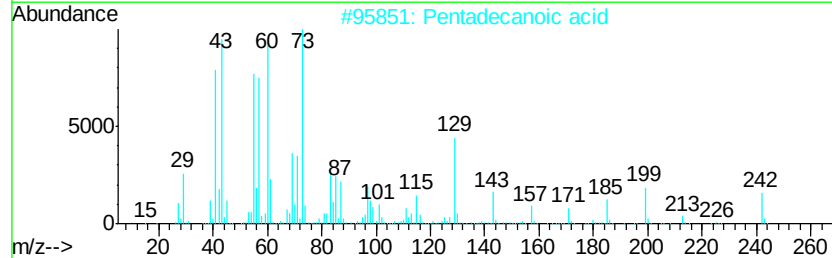
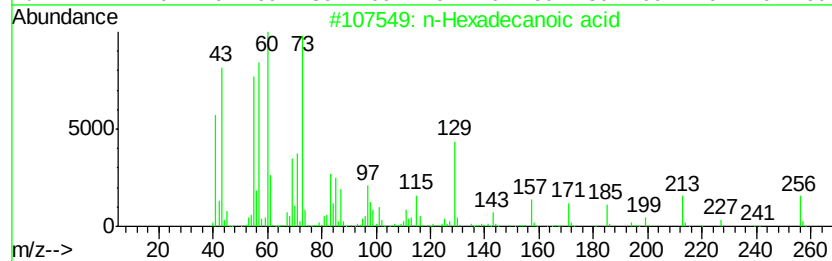
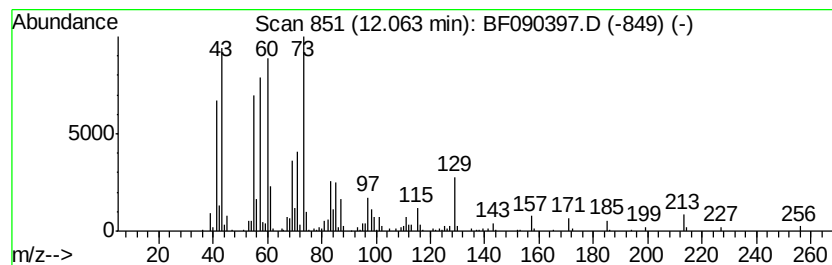
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.06	4.73 ng	535697	Phenanthrene-d10	11.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Undecanoic acid	186	C11H22O2	000112-37-8	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	30



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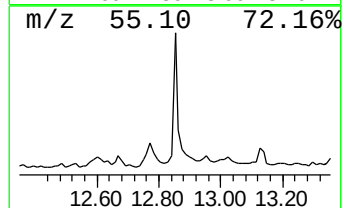
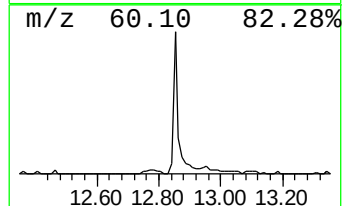
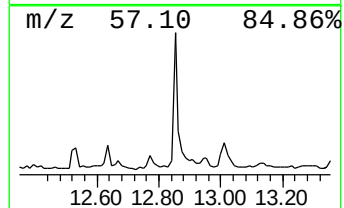
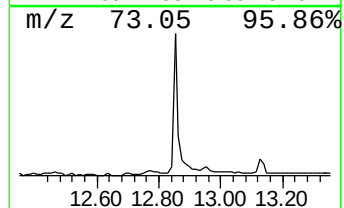
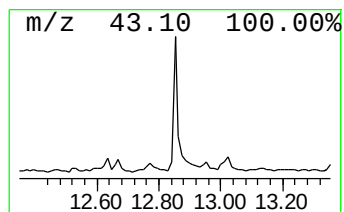
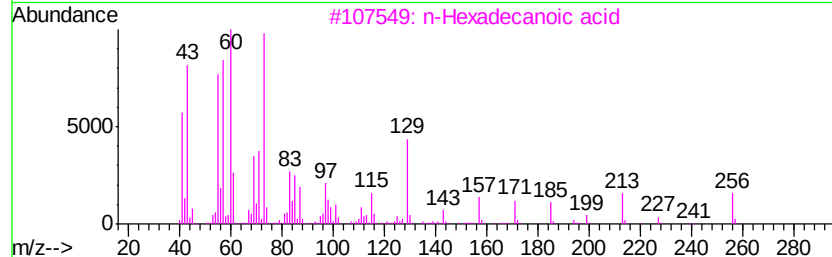
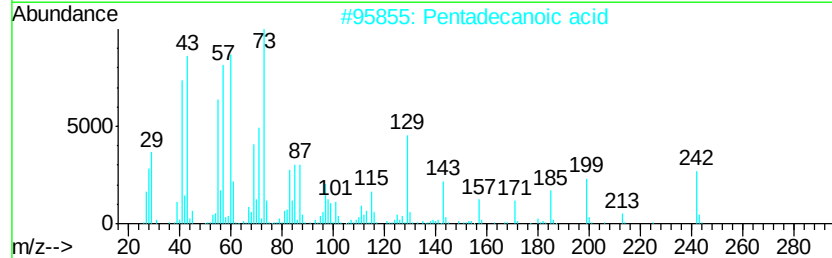
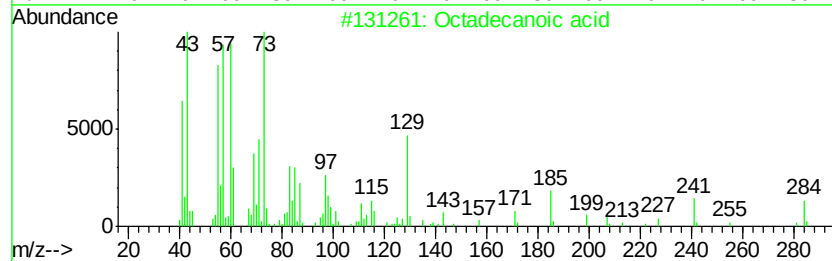
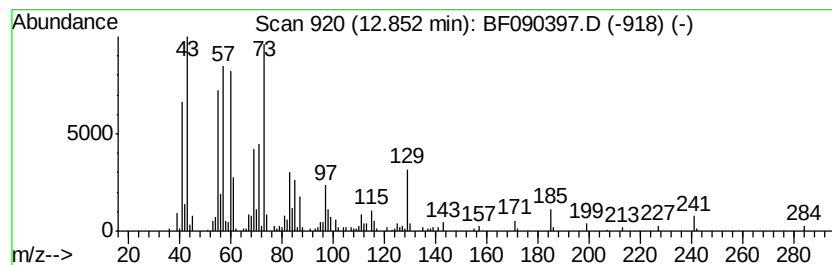
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.85	2.87 ng	324484	Phenanthrene-d10	11.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4		Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	25
5		Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20



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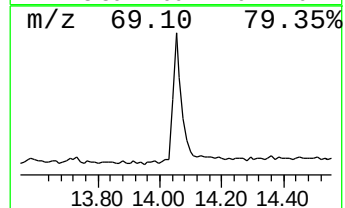
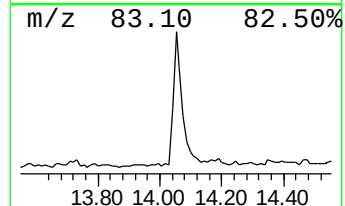
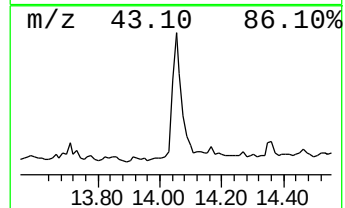
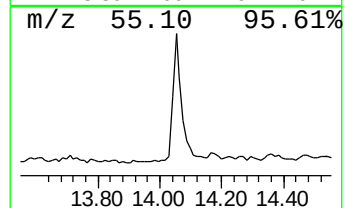
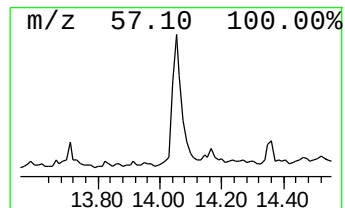
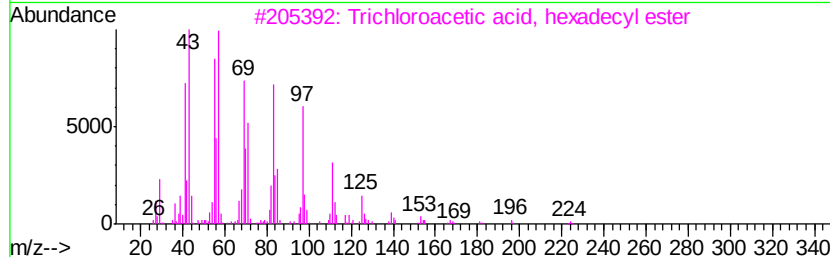
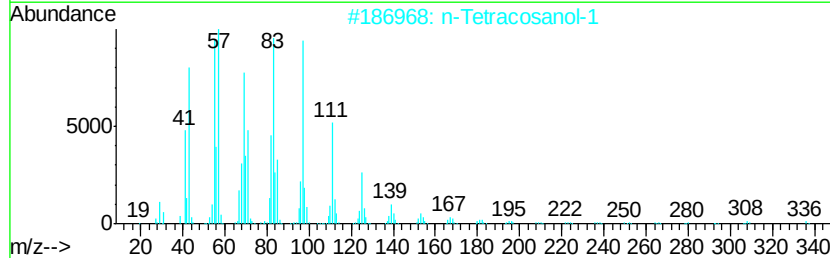
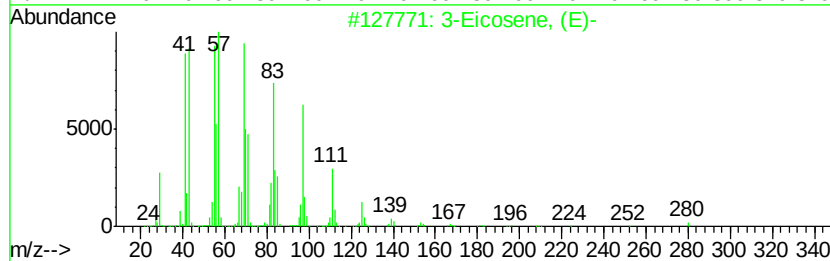
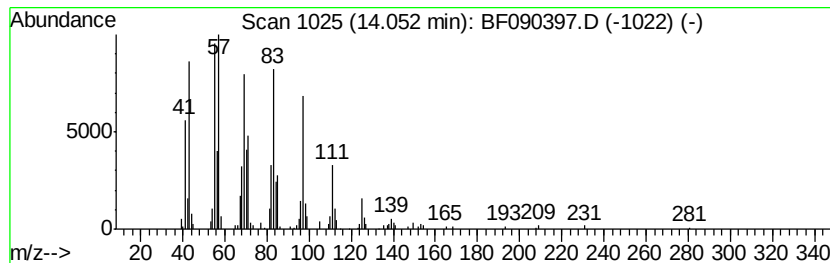
Instrument :
BNA_F
ClientSampleId :
SUP-B003-25-30

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 3-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.05	4.47 ng	404374	Chrysene-d12	14.19	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5	1-Heneicosanol	312	C21H44O	015594-90-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100516\
Data File : BF090397.D
Acq On : 5 Oct 2016 23:18
Operator : UM/SJ
Sample : H5061-19
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B003-25-30

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.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
unknown3.47	3.47	2.4	ng	203252	1	7.00	1719220	20.0
2-Pentanone, 4-hy...	5.21	19.4	ng	1669580	1	7.00	1719220	20.0
unknown6.77	6.77	86.2	ng	7407830	1	7.00	1719220	20.0
n-Hexadecanoic acid	12.06	4.7	ng	535697	4	11.54	2263820	20.0
Octadecanoic acid	12.85	2.9	ng	324484	4	11.54	2263820	20.0
3-Eicosene, (E)-	14.05	4.5	ng	404374	5	14.19	1810410	20.0