

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012417\
 Data File : BF092455.D
 Acq On : 25 Jan 2017 3:20
 Operator : UM/SJ
 Sample : I1397-01
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W-25

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-BF012417.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	5.139	265	267	270	rBV	516116	636702	13.38%	1.745%
2	5.550	301	303	306	rBV	2025570	2266941	47.64%	6.213%
3	6.579	390	393	395	rBV	1879828	1635614	34.37%	4.483%
4	6.727	403	406	409	rBV	3542227	3638077	76.45%	9.971%
5	6.967	424	427	429	rBV	1119769	972985	20.45%	2.667%
6	7.127	438	441	443	rVB	3584609	3597353	75.59%	9.859%
7	7.527	473	476	479	rBV	2213696	3285367	69.04%	9.004%
8	7.962	508	514	516	rBV	140538	229613	4.82%	0.629%
9	8.259	537	540	542	rBV	1478517	1286273	27.03%	3.525%
10	9.345	632	635	638	rBV	4680826	4758961	100.00%	13.043%
11	9.733	667	669	672	rVB	148203	168230	3.54%	0.461%
12	10.031	692	695	696	rBV	1132072	1370672	28.80%	3.756%
13	10.053	696	697	699	rVB	127761	125337	2.63%	0.344%
14	10.442	729	731	737	rVB3	41645	75561	1.59%	0.207%
15	10.545	737	740	744	rBV2	32705	60584	1.27%	0.166%
16	10.671	748	751	755	rVB	219007	327552	6.88%	0.898%
17	10.819	761	764	766	rBV	2514553	2928579	61.54%	8.026%
18	10.865	766	768	770	rVV	225910	309768	6.51%	0.849%
19	10.934	773	774	777	rVB2	66097	79112	1.66%	0.217%
20	11.379	812	813	817	rBV3	45153	86605	1.82%	0.237%
21	11.516	822	825	827	rVV	1166516	1289049	27.09%	3.533%
22	11.722	841	843	848	rVB	48616	80274	1.69%	0.220%
23	12.042	869	871	877	rBV2	286301	322379	6.77%	0.884%
24	12.831	938	940	943	rBV	255000	279623	5.88%	0.766%
25	12.922	946	948	952	rVB2	73923	99824	2.10%	0.274%
26	13.105	961	964	966	rBV	3966397	4049984	85.10%	11.099%
27	13.631	1008	1010	1011	rBV	61146	50874	1.07%	0.139%
28	13.677	1011	1014	1018	rVB	63734	105005	2.21%	0.288%
29	13.997	1040	1042	1047	rBV	119955	132955	2.79%	0.364%
30	14.145	1053	1055	1058	rBV	798334	942967	19.81%	2.584%
31	15.288	1152	1155	1161	rVB	44048	64073	1.35%	0.176%
32	15.631	1181	1185	1187	rBV	577779	852913	17.92%	2.338%
33	15.677	1187	1189	1191	rVB	51577	67080	1.41%	0.184%
34	16.123	1225	1228	1231	rBV	49003	93131	1.96%	0.255%

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Instrument :
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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-BF012417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.648	1270	1274	1281	rVB	42438	92154	1.94%	0.253%
36	17.254	1324	1327	1333	rBV2	25337	58261	1.22%	0.160%
37	17.974	1387	1390	1397	rVB3	22540	67597	1.42%	0.185%

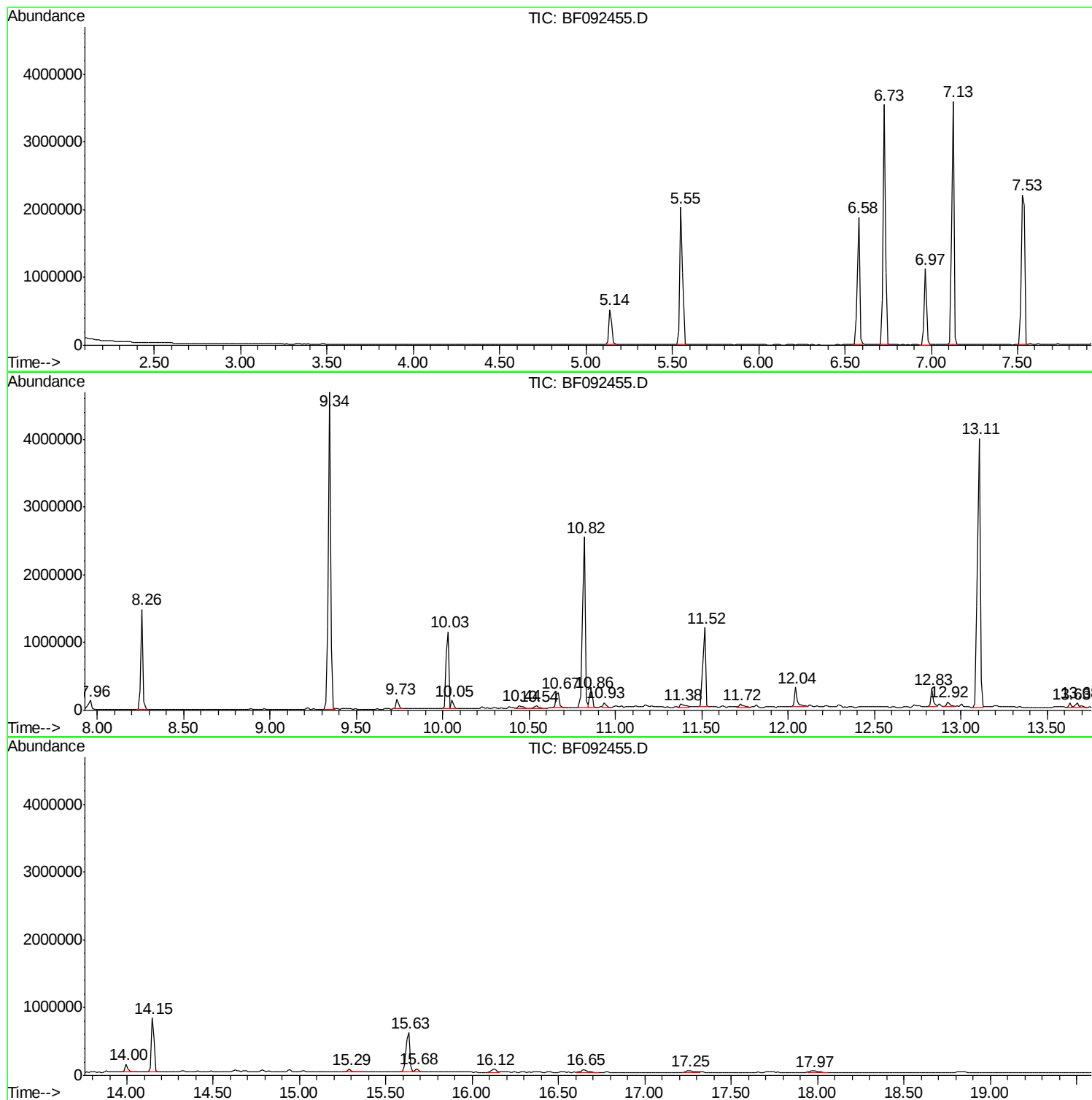
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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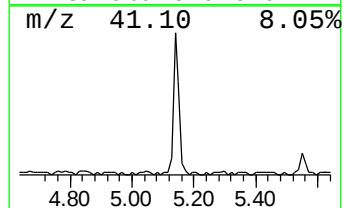
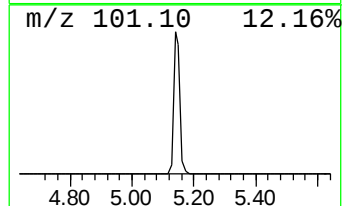
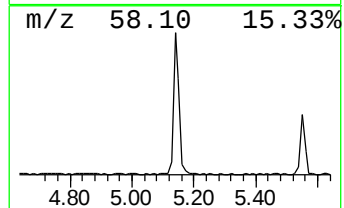
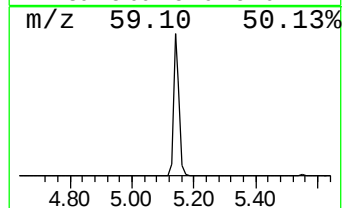
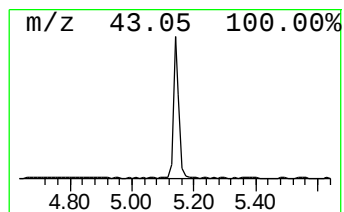
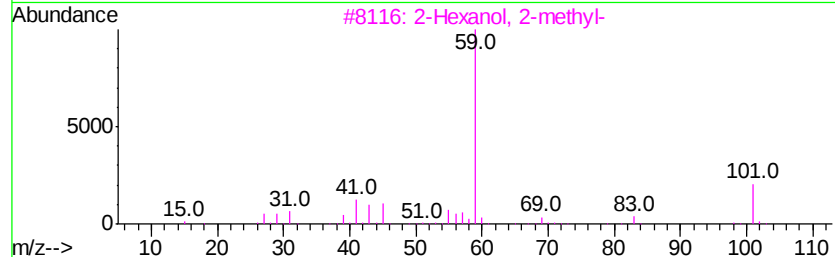
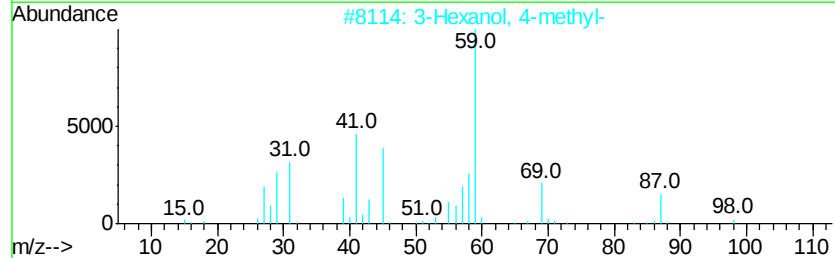
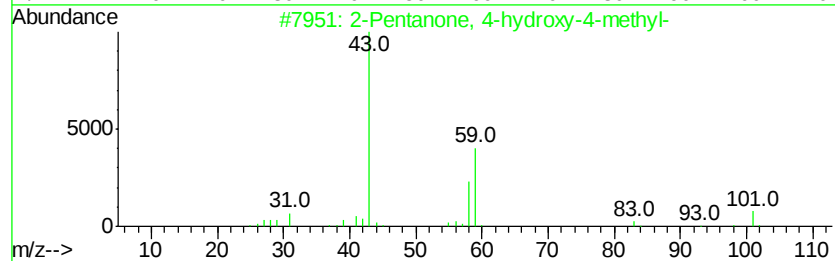
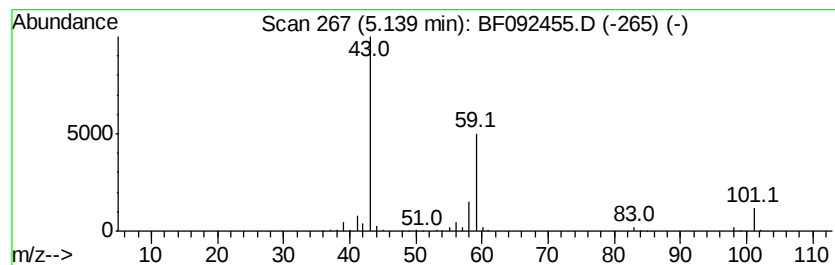
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	13.09 ng	636702	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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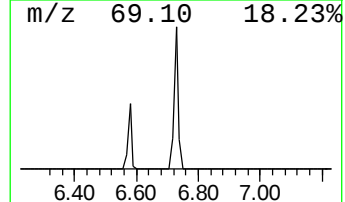
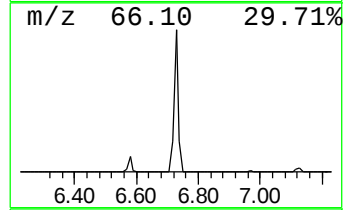
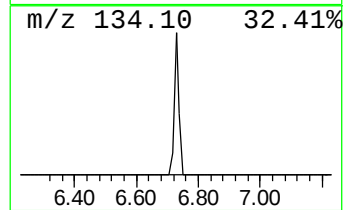
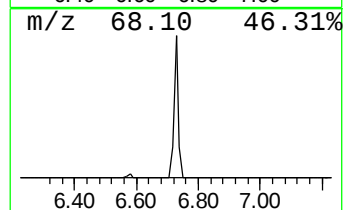
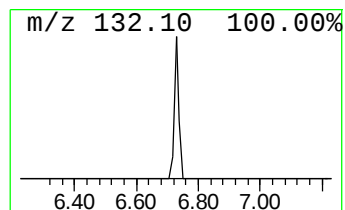
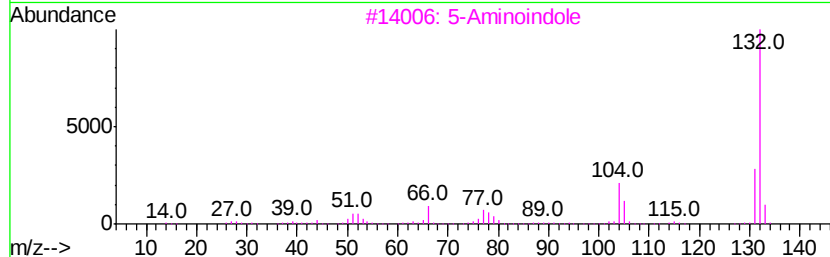
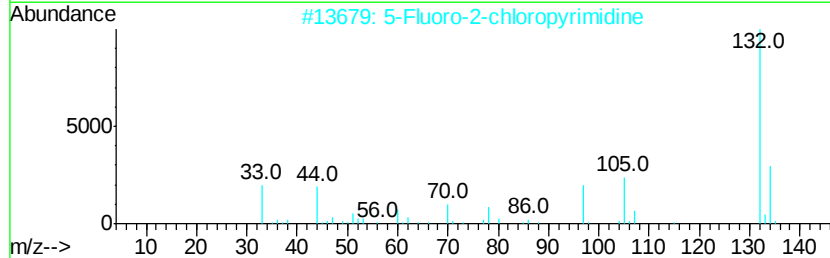
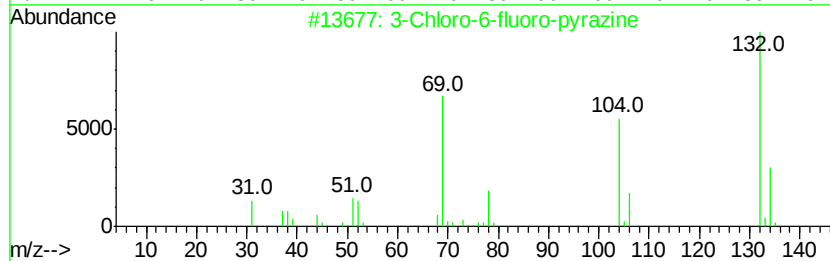
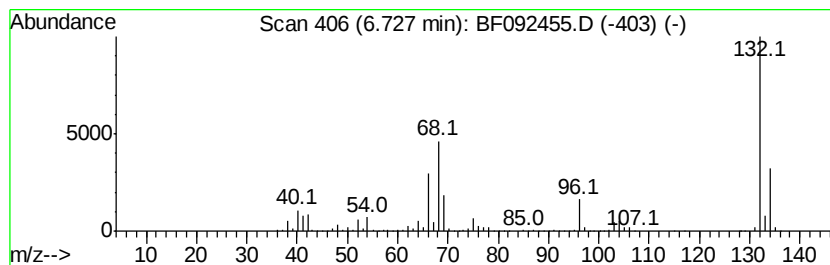
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	74.78 ng	3638080	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
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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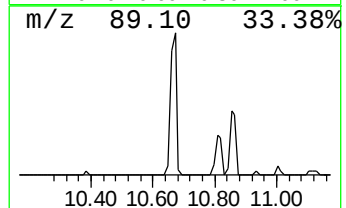
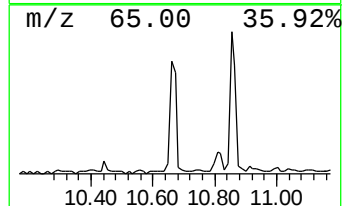
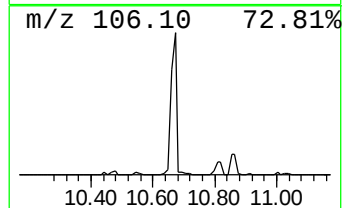
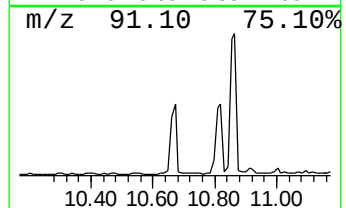
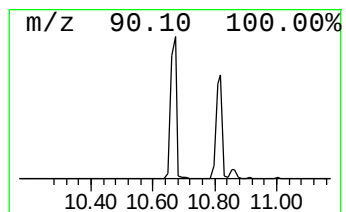
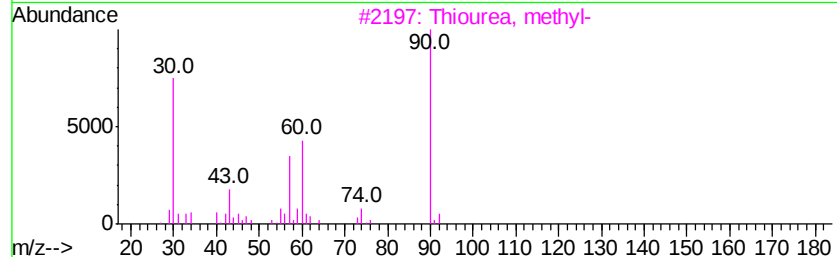
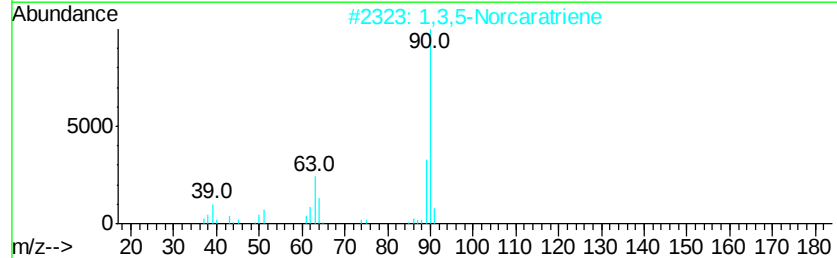
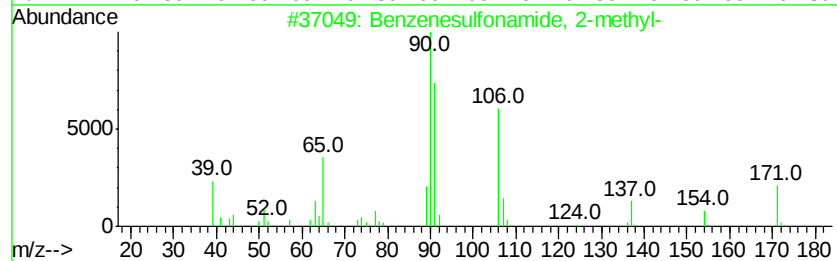
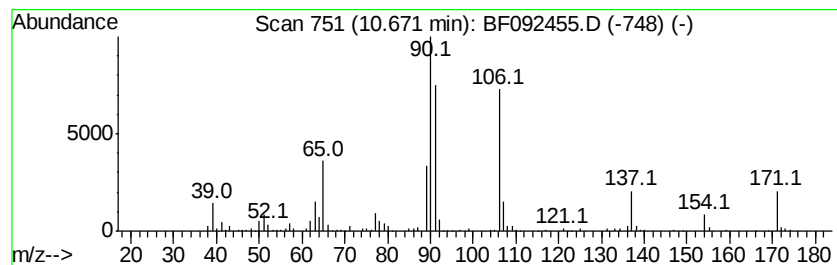
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzenesulfonamide, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	4.78 ng	327552	Acenaphthene-d10	10.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenesulfonamide, 2-methyl-	171	C7H9NO2S	000088-19-7	96
2		1,3,5-Norcaratriene	90	C7H6	004646-69-9	53
3		Thiourea, methyl-	90	C2H6N2S	000598-52-7	33
4		Oxiranecarboxamide, 3-phenyl-	163	C9H9NO2	018538-53-9	9
5		Formic acid, phenylmethyl ester	136	C8H8O2	000104-57-4	9



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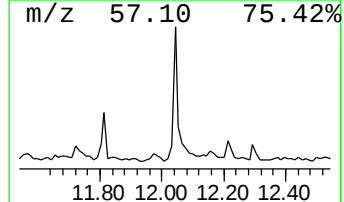
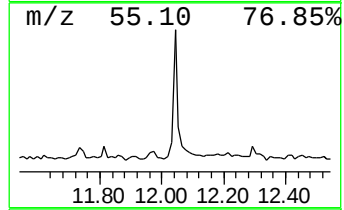
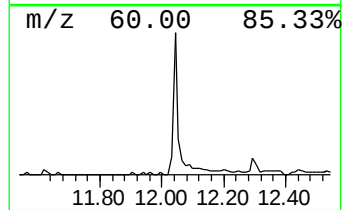
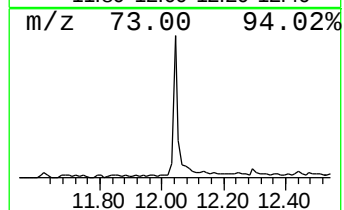
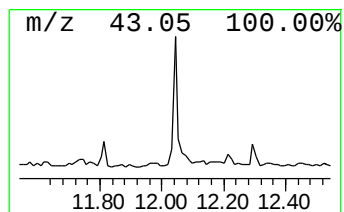
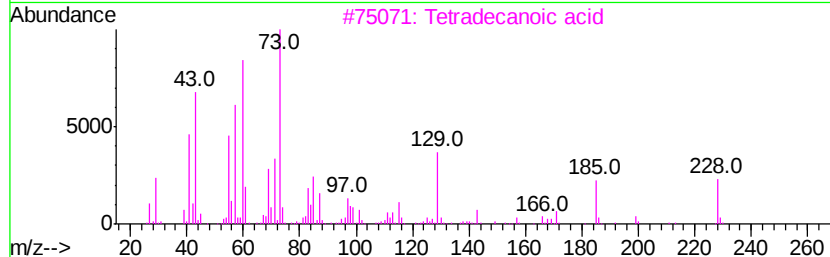
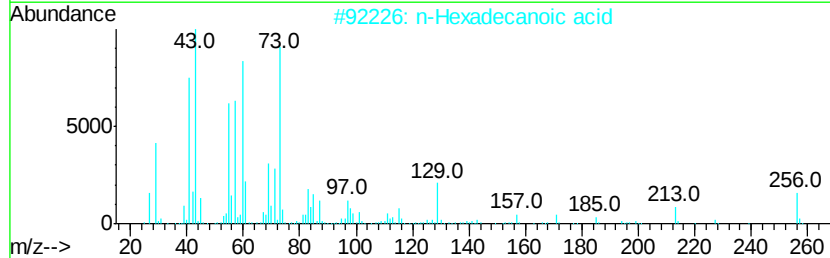
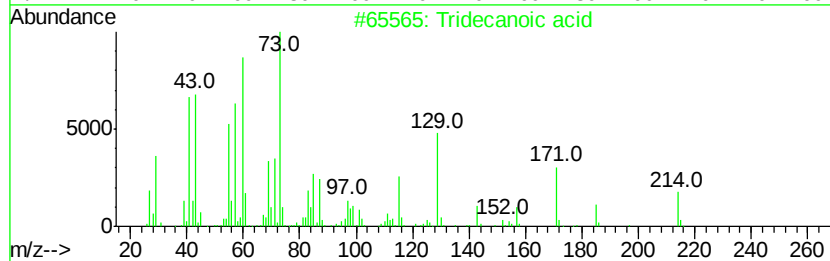
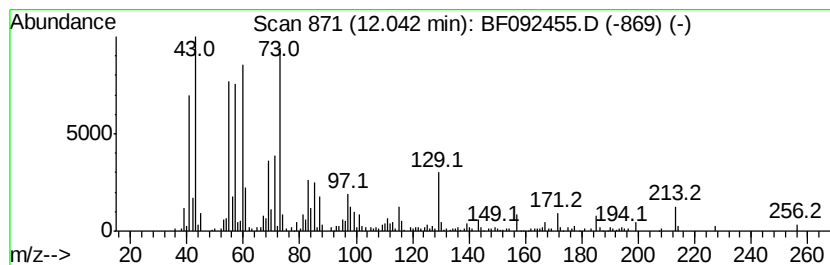
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	5.00 ng	322379	Phenanthrene-d10	11.52

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	94
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4		Undecanoic acid	186	C11H22O2	000112-37-8	64
5		Amyl Nitrite	117	C5H11NO2	000110-46-3	35



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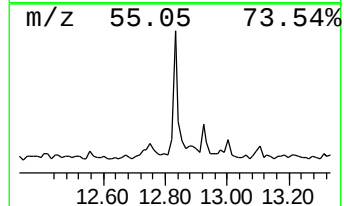
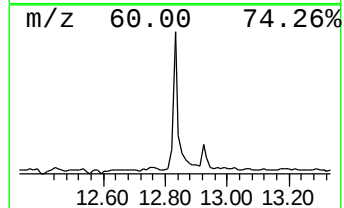
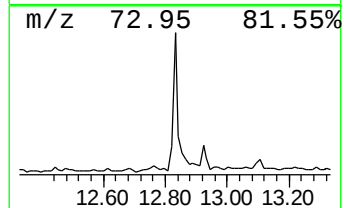
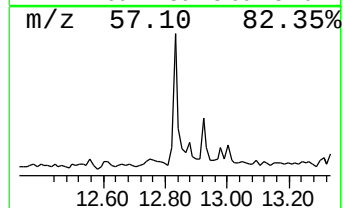
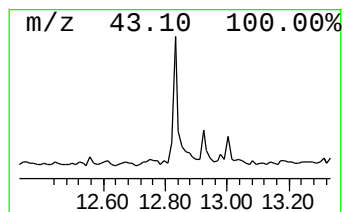
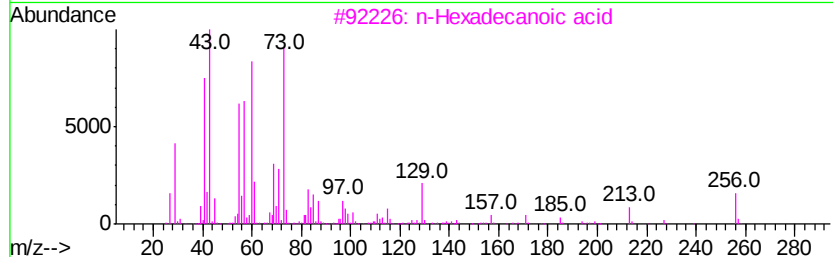
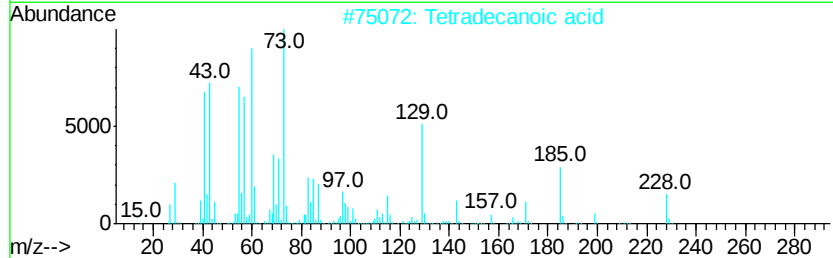
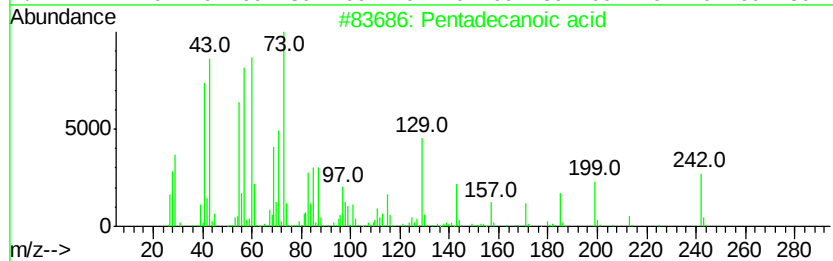
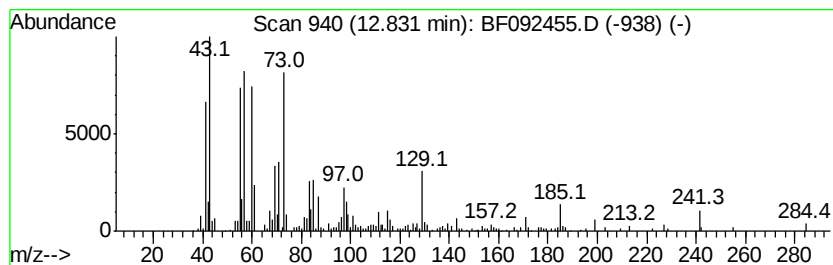
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.83	4.34 ng	279623	Phenanthrene-d10	11.52	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	53
4	Tridecanoic acid	214	C13H26O2	000638-53-9	53
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50



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ClientSampleId :
W-25

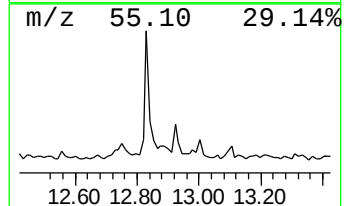
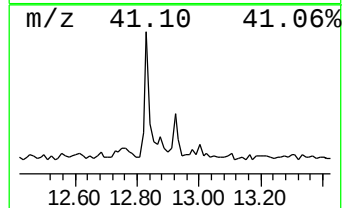
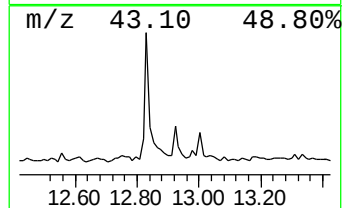
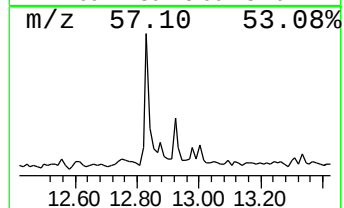
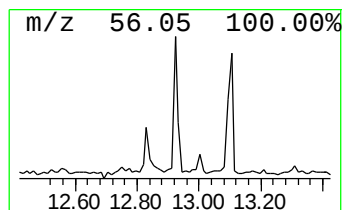
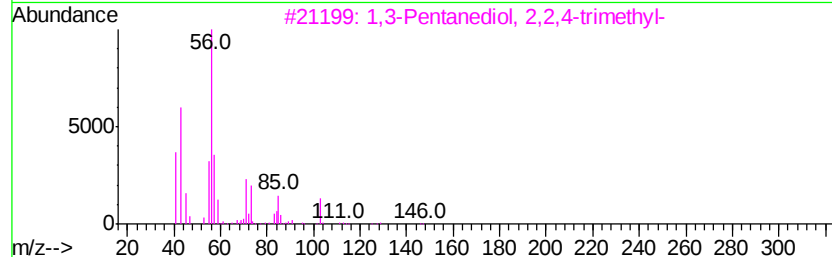
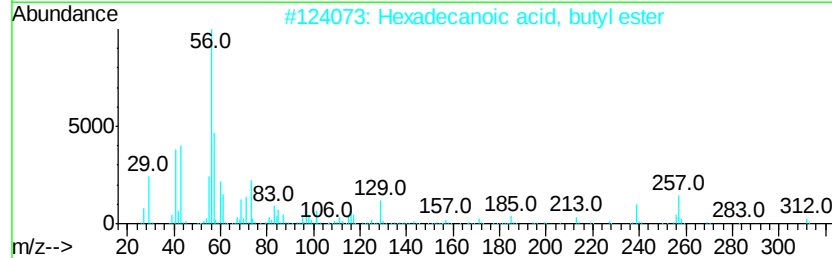
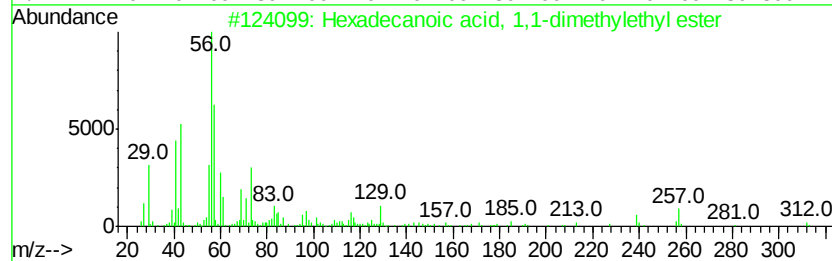
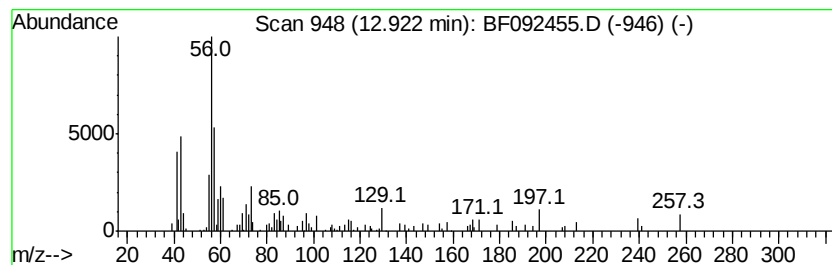
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanoic acid, 1,1-dime... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.92	2.12 ng	99824	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	87
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	78
3		1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	50
4		2-Decene, 9-methyl-, (Z)-	154	C11H22	074630-24-3	38
5		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012417\
Data File : BF092455.D
Acq On : 25 Jan 2017 3:20
Operator : UM/SJ
Sample : I1397-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

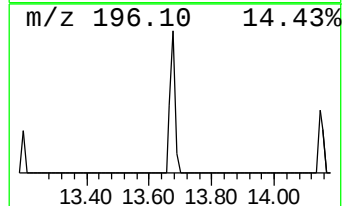
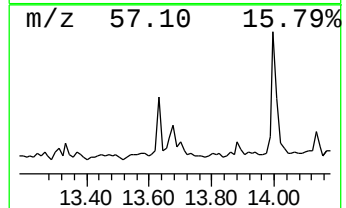
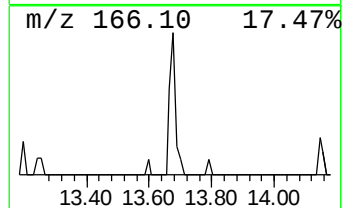
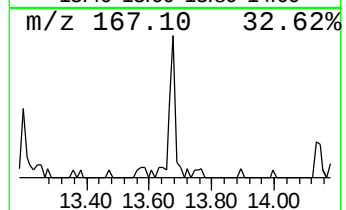
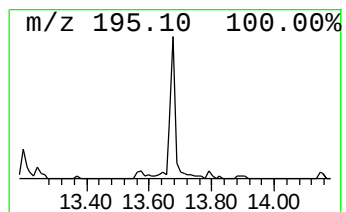
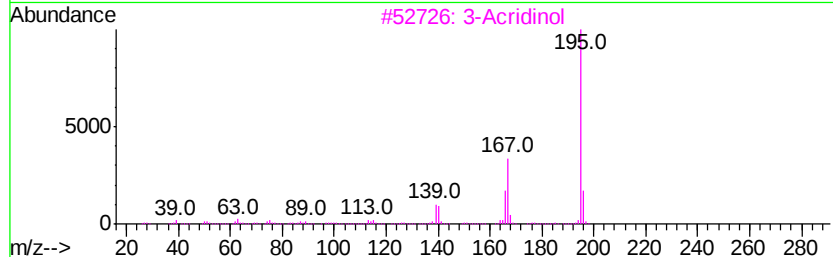
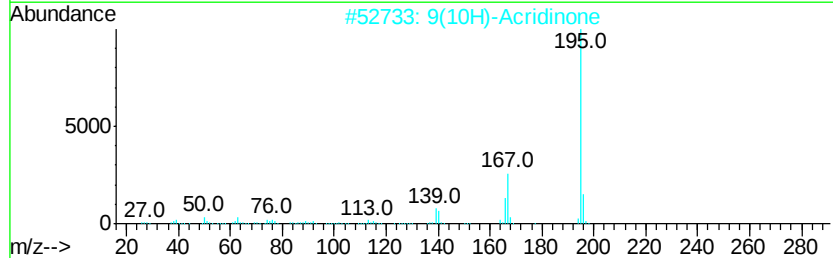
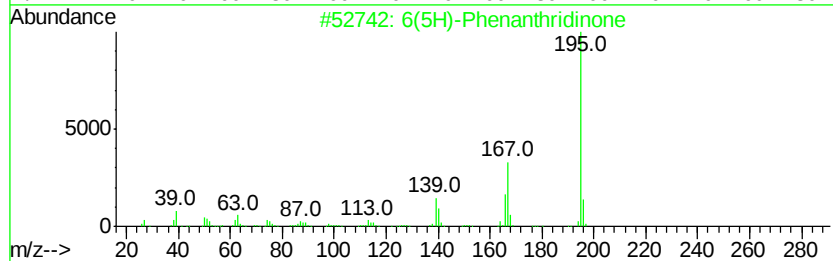
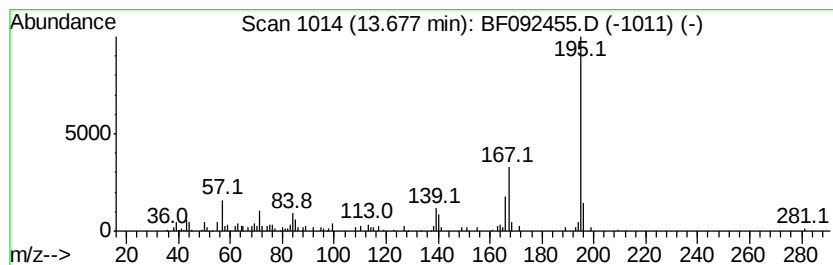
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 6(5H)-Phenanthridinone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.68	2.23 ng	105005	Chrysene-d12	14.15		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6(5H)-Phenanthridinone	195	C13H9NO	001015-89-0	95	
2	9(10H)-Acridinone	195	C13H9NO	000578-95-0	95	
3	3-Acridinol	195	C13H9NO	007132-70-9	94	
4	4-Amino-9-fluorenone	195	C13H9NO	004269-15-2	93	
5	8-Methyl-4-azafluorenone	195	C13H9NO	064292-03-1	90	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012417\
Data File : BF092455.D
Acq On : 25 Jan 2017 3:20
Operator : UM/SJ
Sample : I1397-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

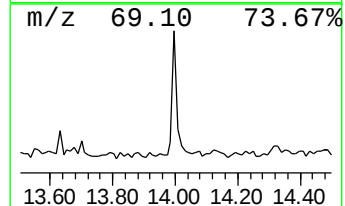
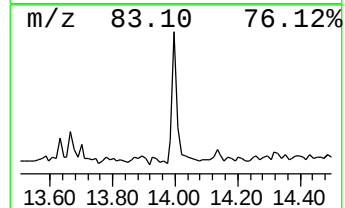
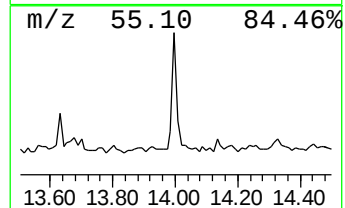
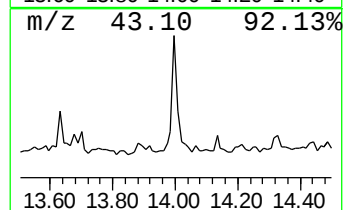
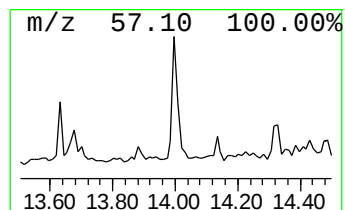
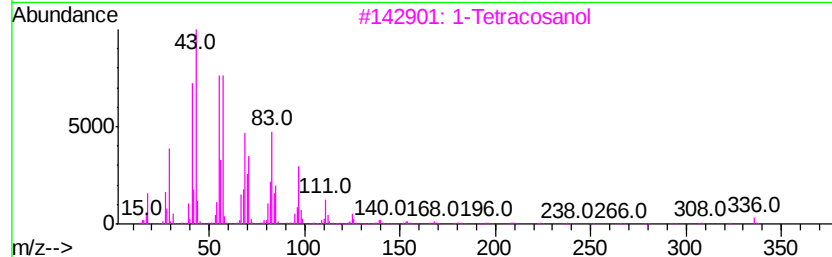
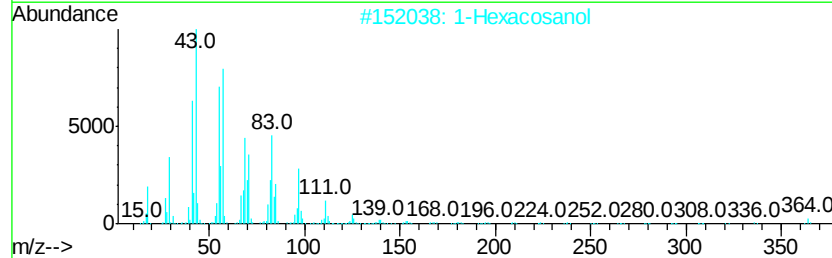
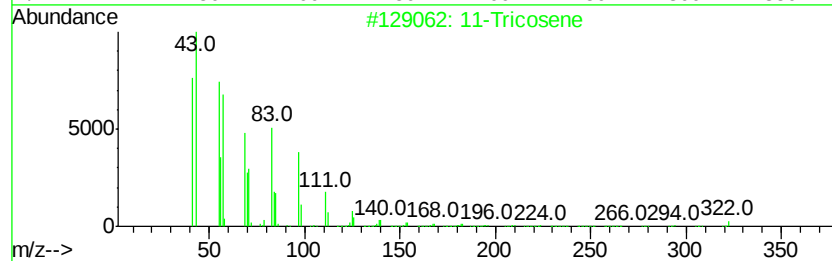
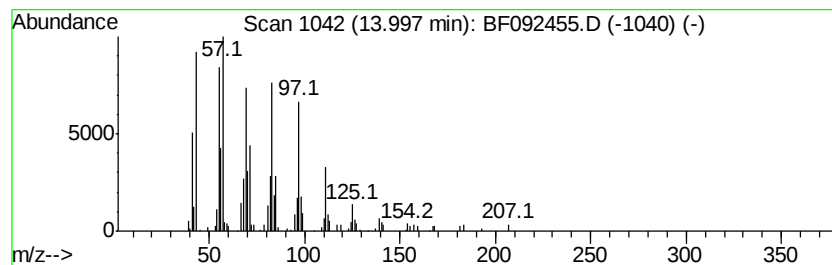
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 11-Tricosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.00	2.82 ng	132955	Chrysene-d12		14.15
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Tricosene	322	C23H46	052078-56-5	90
2	1-Hexacosanol	382	C26H54O	000506-52-5	83
3	1-Tetracosanol	354	C24H50O	000506-51-4	83
4	1-Heptadecanol	256	C17H36O	001454-85-9	80
5	1-Docosene	308	C22H44	001599-67-3	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012417\
Data File : BF092455.D
Acq On : 25 Jan 2017 3:20
Operator : UM/SJ
Sample : I1397-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-25

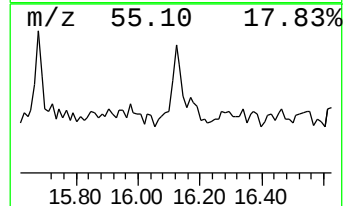
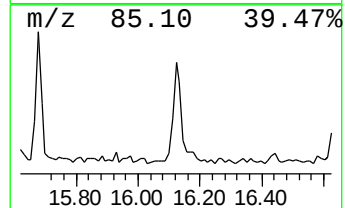
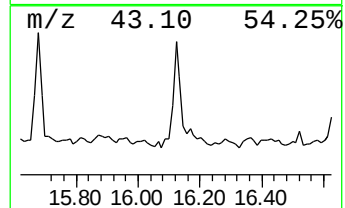
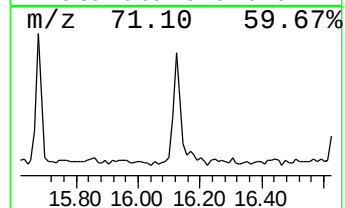
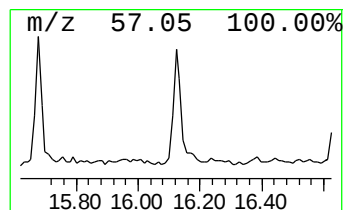
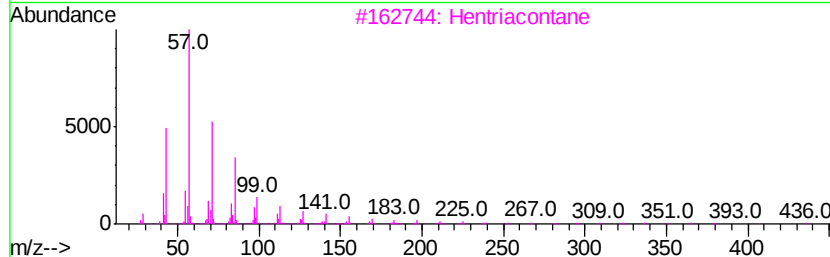
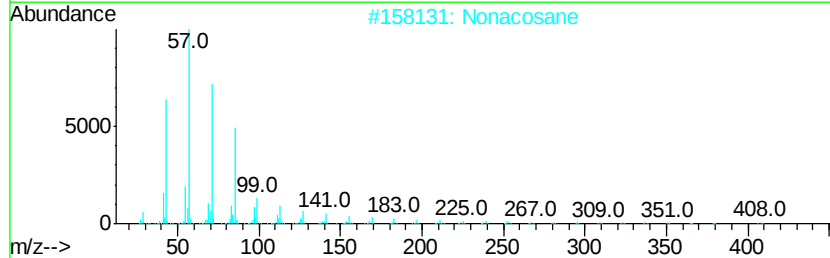
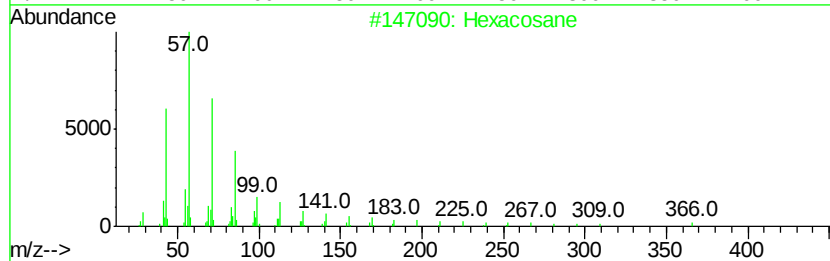
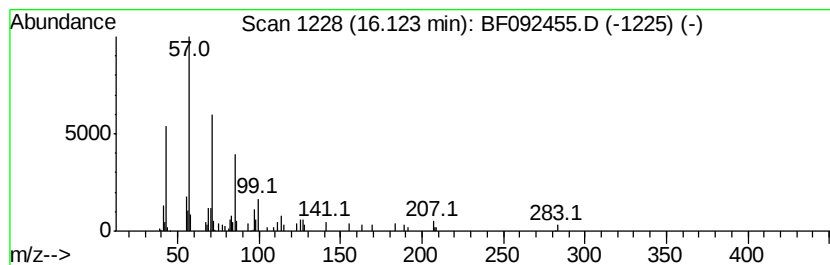
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.12	2.18 ng	93131	Perylene-d12	15.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Nonacosane	408	C29H60	000630-03-5	90
3		Hentriacontane	437	C31H64	000630-04-6	90
4		Pentacosane	352	C25H52	000629-99-2	87
5		Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012417\
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Acq On : 25 Jan 2017 3:20
Operator : UM/SJ
Sample : I1397-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

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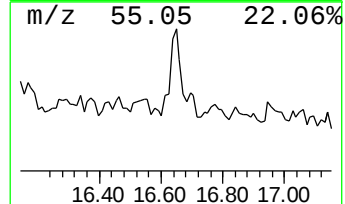
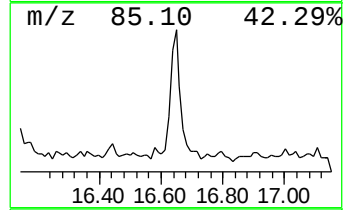
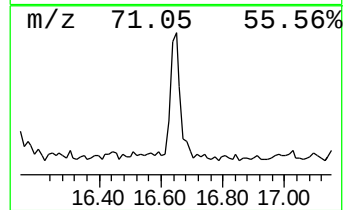
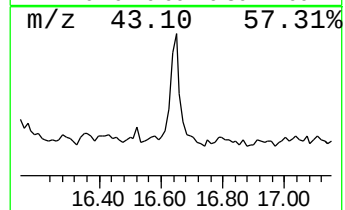
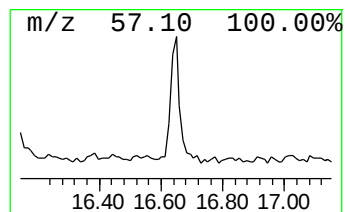
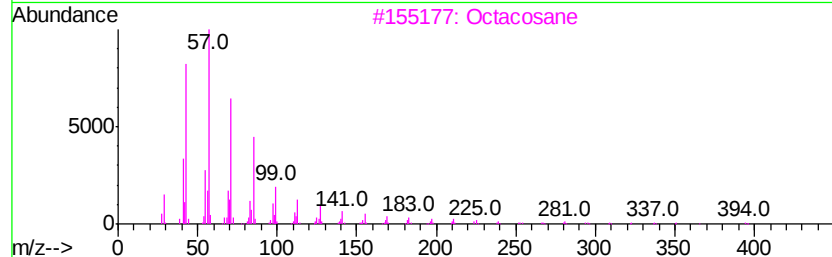
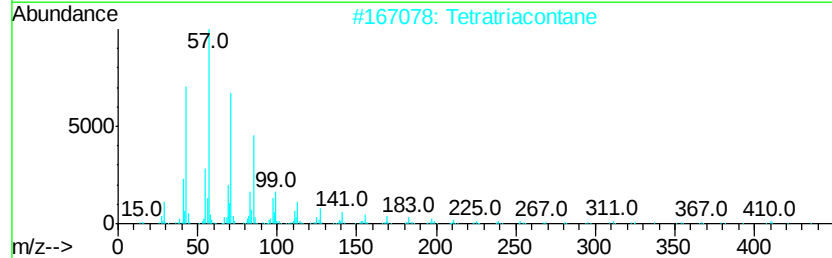
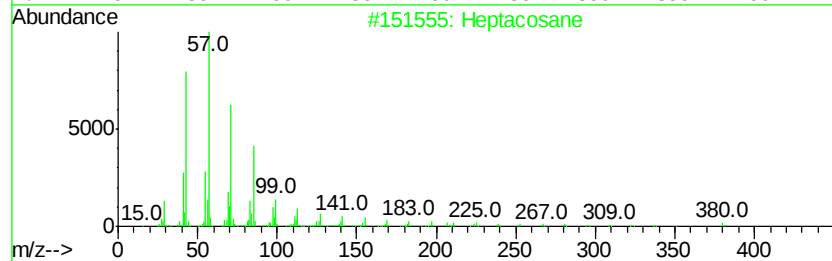
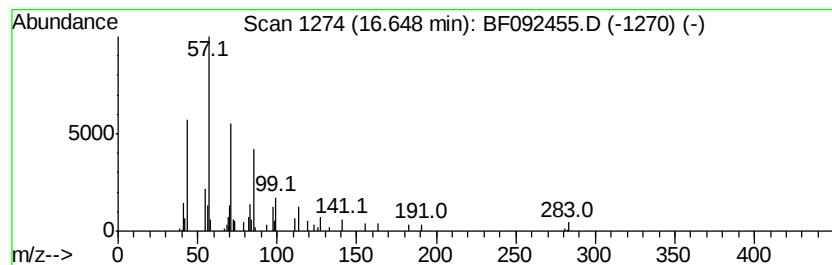
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.65	2.16 ng	92154	Perylene-d12	15.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	90
2			Tetratriacontane	479	C34H70	014167-59-0	87
3			Octacosane	394	C28H58	000630-02-4	87
4			Tetratetracontane	619	C44H90	007098-22-8	86
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012417\
 Data File : BF092455.D
 Acq On : 25 Jan 2017 3:20
 Operator : UM/SJ
 Sample : I1397-01
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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...	5.14	13.1	ng	636702	1	6.97	972985	20.0
unknown6.73	6.73	74.8	ng	3638080	1	6.97	972985	20.0
Benzenesulfonamid...	10.67	4.8	ng	327552	3	10.03	1370670	20.0
Tridecanoic acid	12.04	5.0	ng	322379	4	11.52	1289050	20.0
Pentadecanoic acid	12.83	4.3	ng	279623	4	11.52	1289050	20.0
Hexadecanoic acid...	12.92	2.1	ng	99824	5	14.15	942967	20.0
6(5H)-Phenanthrid...	13.68	2.2	ng	105005	5	14.15	942967	20.0
11-Tricosene	14.00	2.8	ng	132955	5	14.15	942967	20.0
Hexacosane	16.12	2.2	ng	93131	6	15.63	852913	20.0
Heptacosane	16.65	2.2	ng	92154	6	15.63	852913	20.0