

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012417\
 Data File : BF092458.D
 Acq On : 25 Jan 2017 4:42
 Operator : UM/SJ
 Sample : I1397-04
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W-12

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	5.138	265	267	270	rBV	403235	568896	12.49%	1.371%
2	5.550	301	303	306	rBV	1939815	2360024	51.81%	5.687%
3	6.579	390	393	395	rBV	1885232	1633620	35.86%	3.936%
4	6.727	403	406	409	rBV	3543982	3634253	79.78%	8.757%
5	6.967	424	427	429	rBV	1116361	1001424	21.98%	2.413%
6	7.127	438	441	443	rVB	3362937	3524639	77.38%	8.493%
7	7.527	473	476	479	rBV	2096264	3220878	70.71%	7.761%
8	8.259	538	540	542	rBV	1503476	1305198	28.65%	3.145%
9	8.979	600	603	608	rBV	75596	114540	2.51%	0.276%
10	9.093	611	613	615	rBV	53253	57568	1.26%	0.139%
11	9.230	622	625	630	rVB5	56046	90269	1.98%	0.218%
12	9.345	632	635	638	rVV	4410246	4555253	100.00%	10.977%
13	9.630	657	660	661	rBV2	28738	58910	1.29%	0.142%
14	9.733	667	669	671	rVB	151754	171407	3.76%	0.413%
15	9.973	688	690	692	rVB2	45149	52806	1.16%	0.127%
16	10.030	692	695	697	rBV	968790	1376911	30.23%	3.318%
17	10.156	705	706	709	rBV2	49082	71321	1.57%	0.172%
18	10.213	709	711	715	rVV4	39710	68508	1.50%	0.165%
19	10.305	717	719	721	rVV3	40935	57334	1.26%	0.138%
20	10.350	721	723	726	rVV3	38037	72743	1.60%	0.175%
21	10.545	738	740	741	rVB	53302	51520	1.13%	0.124%
22	10.602	744	745	747	rBV2	31838	46269	1.02%	0.111%
23	10.693	747	753	755	rVV	2491672	3749428	82.31%	9.035%
24	10.819	761	764	766	rBV	2514519	2783650	61.11%	6.708%
25	10.899	766	771	773	rVV	2205599	3770614	82.78%	9.086%
26	10.933	773	774	778	rVB2	63526	76007	1.67%	0.183%
27	11.002	778	780	781	rBV2	73449	67535	1.48%	0.163%
28	11.185	794	796	797	rVB	41996	50379	1.11%	0.121%
29	11.219	797	799	801	rBV	36122	54737	1.20%	0.132%
30	11.516	822	825	827	rVB	1317374	1243611	27.30%	2.997%
31	11.711	840	842	843	rBV	46032	45558	1.00%	0.110%
32	11.802	848	850	852	rVB	53069	73962	1.62%	0.178%
33	12.042	869	871	876	rBV3	121513	227418	4.99%	0.548%
34	12.831	938	940	943	rBV2	93892	115134	2.53%	0.277%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012417\
Data File : BF092458.D
Acq On : 25 Jan 2017 4:42
Operator : UM/SJ
Sample : I1397-04
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-12

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	12.991	952	954	959	rVB	73340	86726	1.90%	0.209%
36	13.105	961	964	966	rBV	3163717	3038233	66.70%	7.321%
37	13.676	1012	1014	1016	rBV	50800	64688	1.42%	0.156%
38	13.996	1040	1042	1045	rBV	83773	86387	1.90%	0.208%
39	14.157	1053	1056	1058	rBV	837122	845174	18.55%	2.037%
40	15.631	1182	1185	1188	rBV	666603	852827	18.72%	2.055%
41	15.677	1188	1189	1202	rVB5	34644	96858	2.13%	0.233%
42	16.648	1271	1274	1284	rVB6	22590	76111	1.67%	0.183%

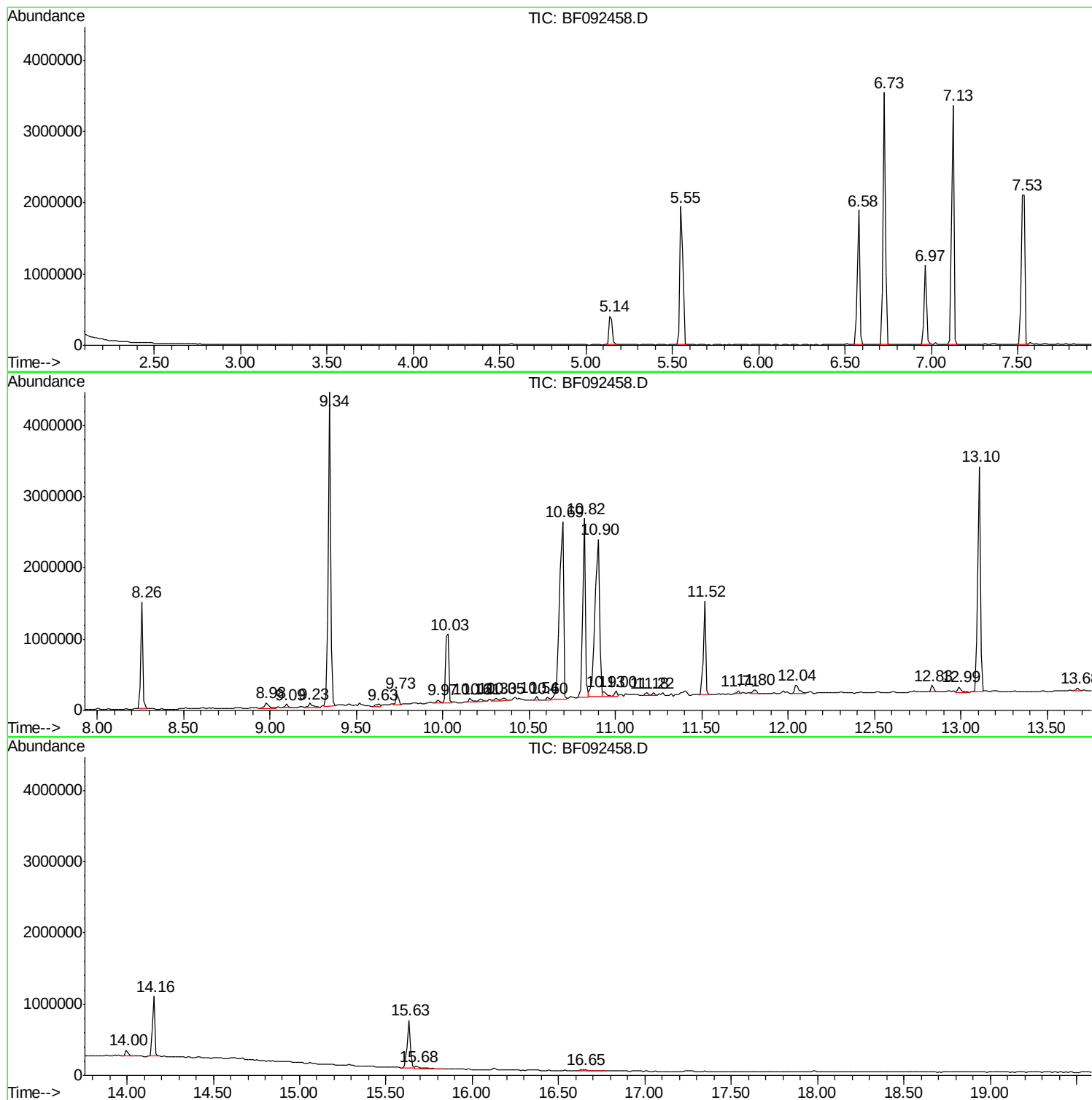
Sum of corrected areas: 41499328

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012417\
Data File : BF092458.D
Acq On : 25 Jan 2017 4:42
Operator : UM/SJ
Sample : I1397-04
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-12

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012417\
Data File : BF092458.D
Acq On : 25 Jan 2017 4:42
Operator : UM/SJ
Sample : I1397-04
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-12

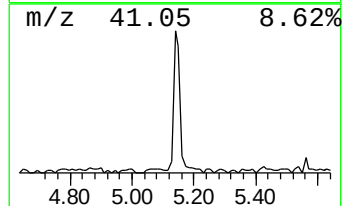
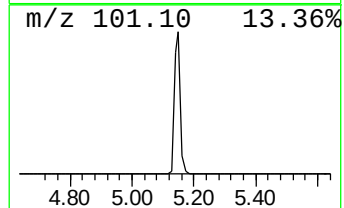
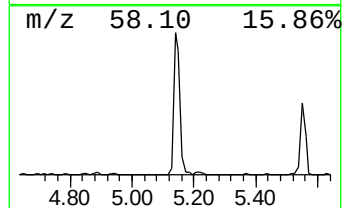
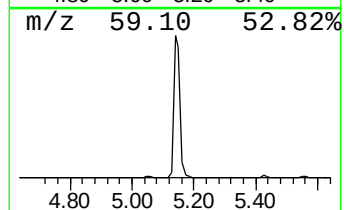
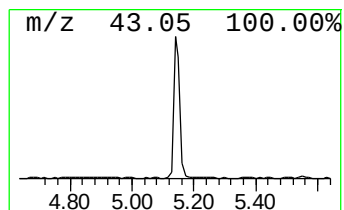
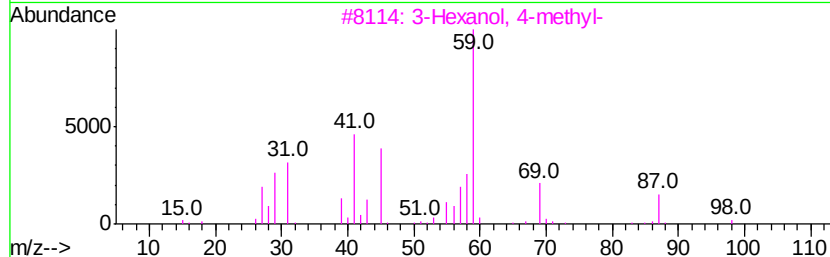
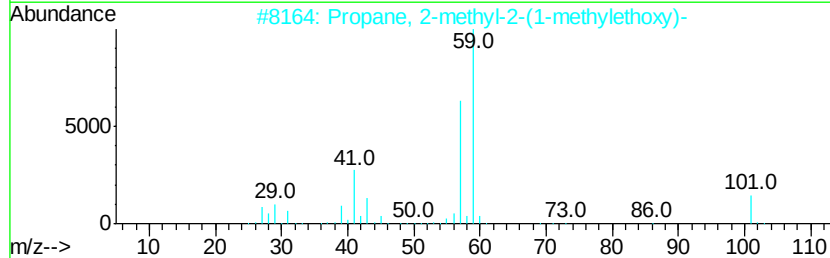
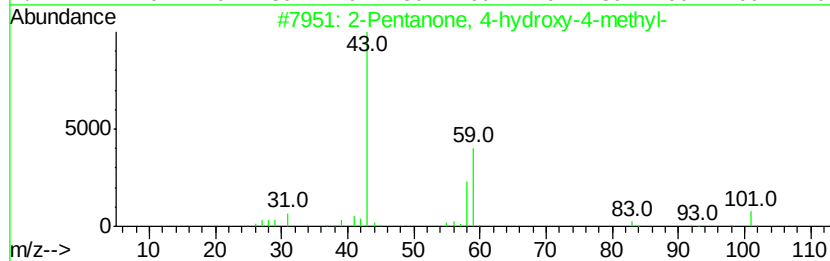
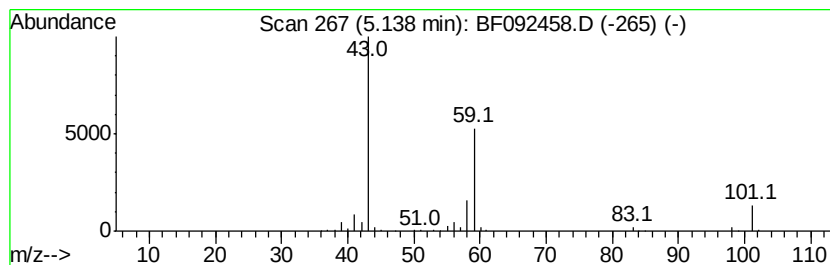
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	11.36 ng	568896	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	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012417\
Data File : BF092458.D
Acq On : 25 Jan 2017 4:42
Operator : UM/SJ
Sample : I1397-04
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-12

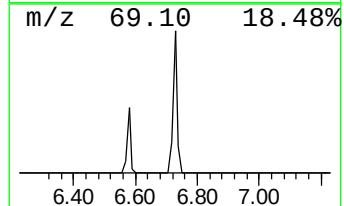
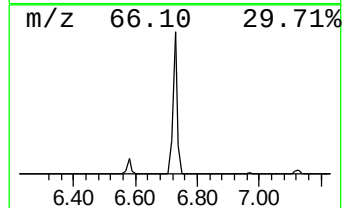
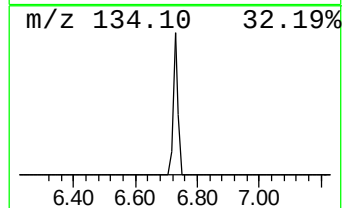
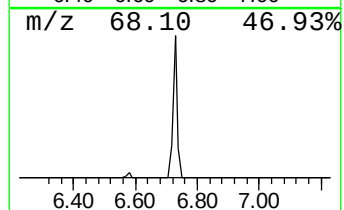
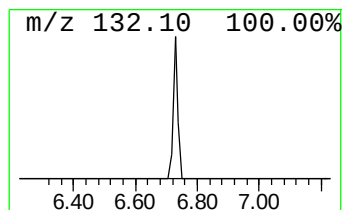
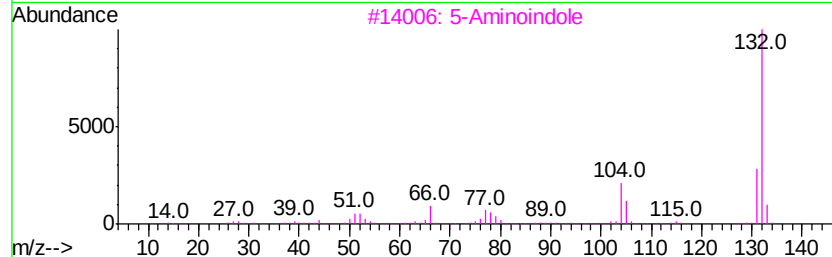
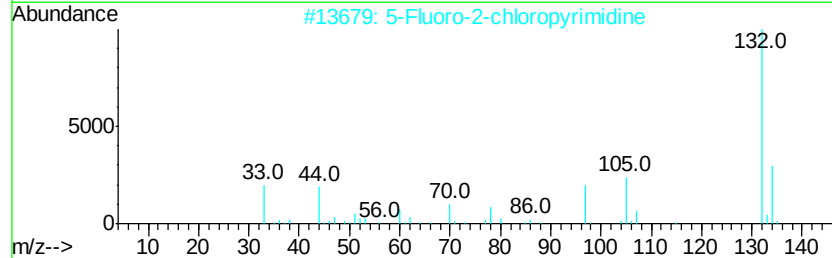
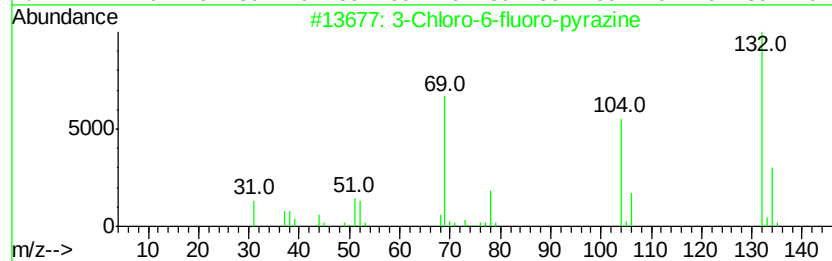
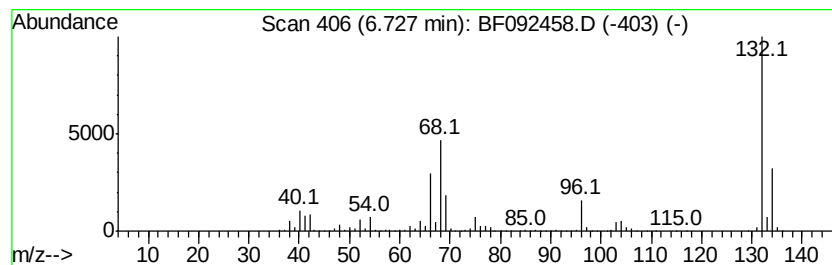
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	72.58 ng	3634250	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	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012417\
Data File : BF092458.D
Acq On : 25 Jan 2017 4:42
Operator : UM/SJ
Sample : I1397-04
Misc :
ALS Vial : 39 Sample Multiplier: 1

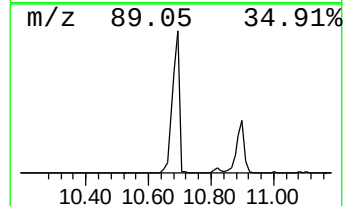
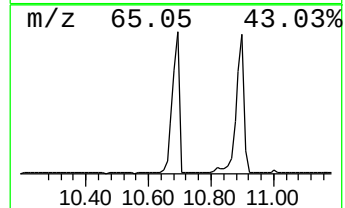
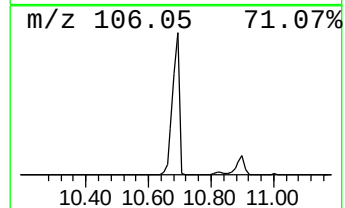
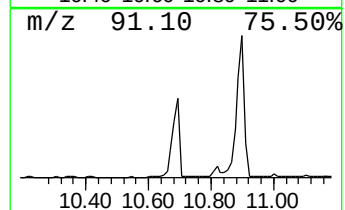
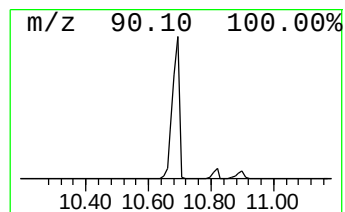
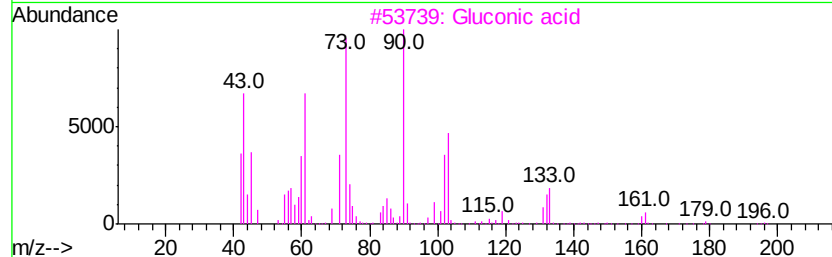
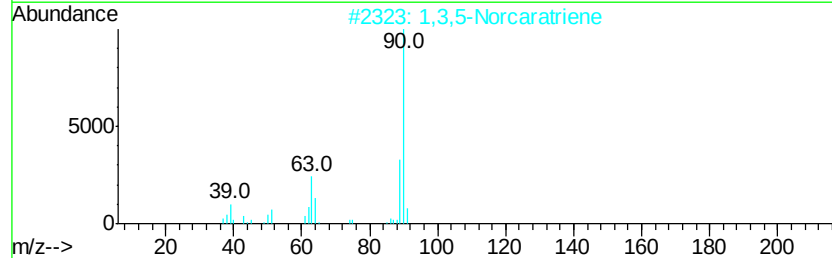
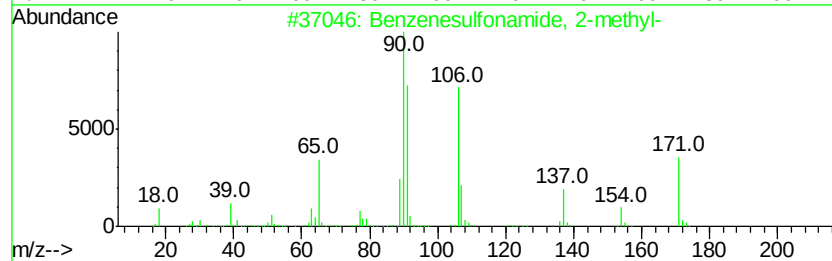
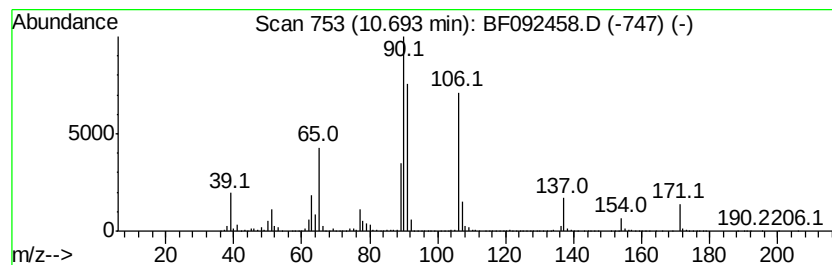
Instrument :
BNA_F
ClientSampleId :
W-12

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 4 Benzenesulfonamide, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.69	54.46 ng	3749430	Acenaphthene-d10		10.03
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 2-methyl-	171	C7H9NO2S	000088-19-7	97
2	1,3,5-Norcaratriene	90	C7H6	004646-69-9	46
3	Gluconic acid	196	C6H12O7	000526-95-4	38
4	Benzene, 1-methyl-3-nitro-	137	C7H7NO2	000099-08-1	30
5	Thiourea, methyl-	90	C2H6N2S	000598-52-7	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012417\
Data File : BF092458.D
Acq On : 25 Jan 2017 4:42
Operator : UM/SJ
Sample : I1397-04
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-12

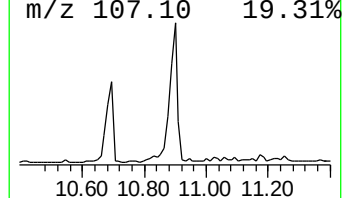
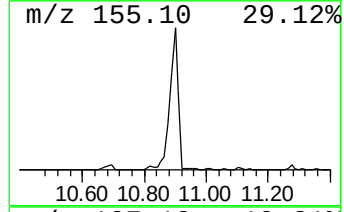
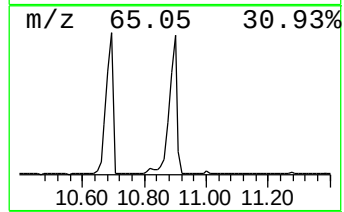
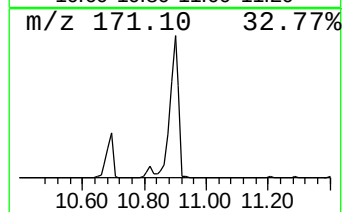
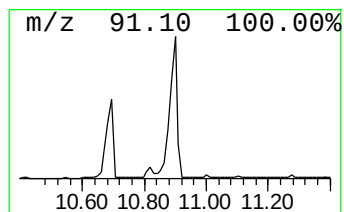
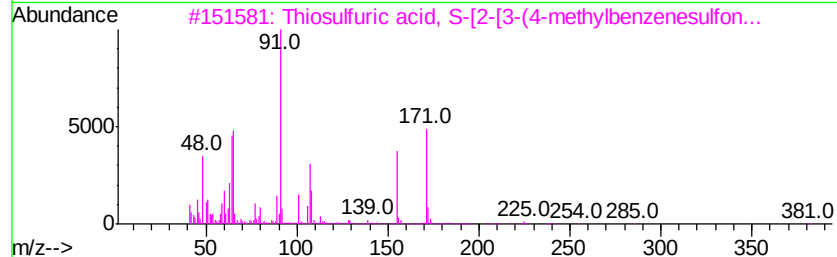
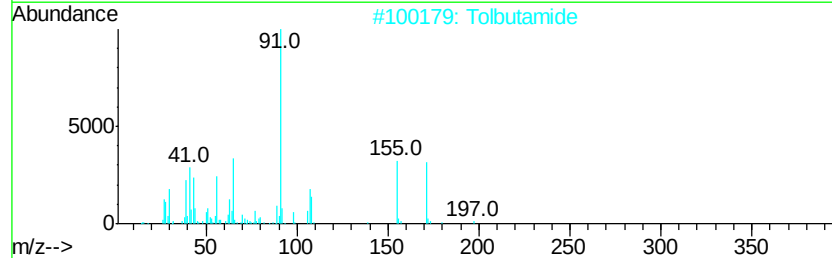
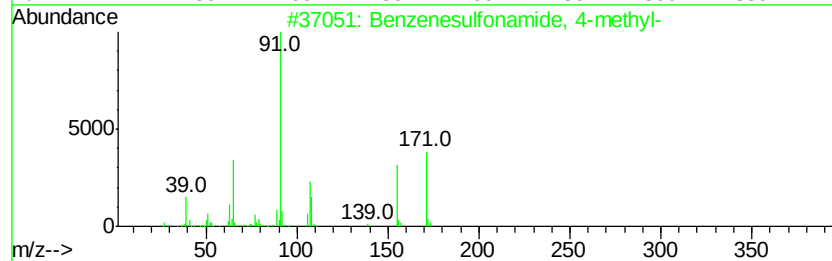
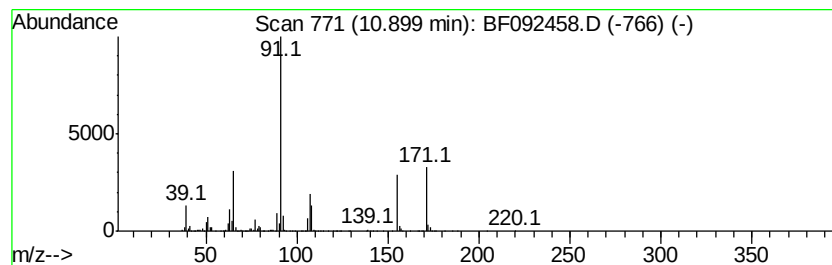
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzenesulfonamide, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	60.64 ng	3770610	Phenanthrene-d10	11.52

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	98
2		Tolbutamide	270	C12H18N2O3S	000064-77-7	91
3		Thiosulfuric acid, S-[2-[3-(4-methyl-...]	381	C12H19N3O5S3	1000255-60-3	80
4		O-p-toluenesulfonyl-N-acetylserine	315	C13H17NO6S	1000126-44-8	72
5		N-p-toluenesulfonyl-L-threonine,...	363	C18H21NO5S	1000130-34-4	68



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012417\
Data File : BF092458.D
Acq On : 25 Jan 2017 4:42
Operator : UM/SJ
Sample : I1397-04
Misc :
ALS Vial : 39 Sample Multiplier: 1

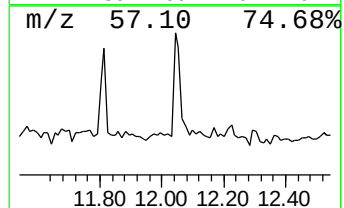
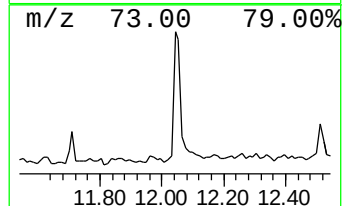
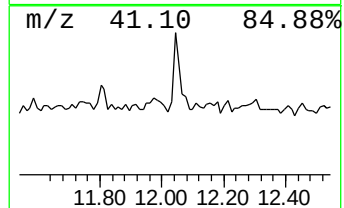
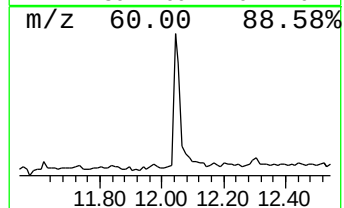
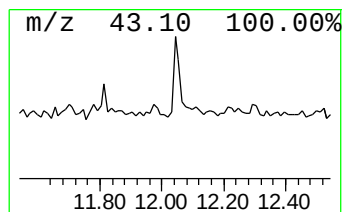
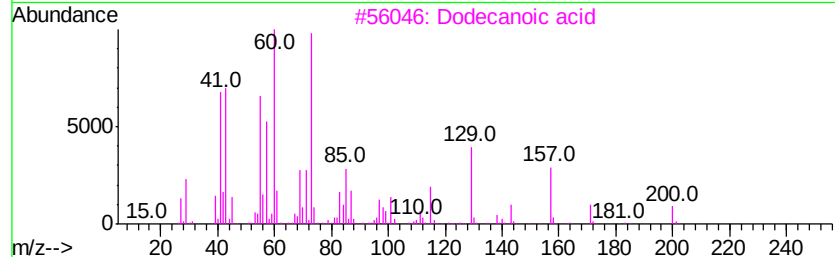
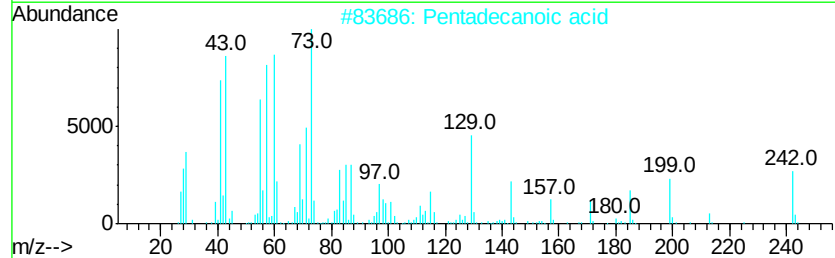
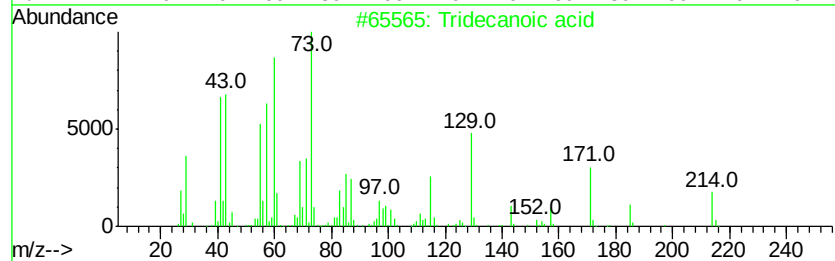
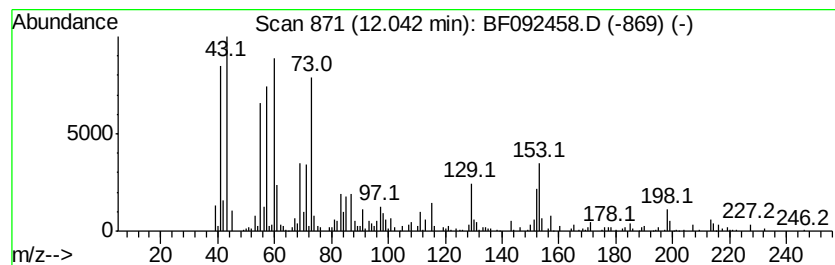
Instrument :
BNA_F
ClientSampleId :
W-12

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 6 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.04	3.66 ng	227418	Phenanthrene-d10		11.52
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	83
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Dodecanoic acid	200	C12H24O2	000143-07-7	49
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	47
5	Undecanoic acid	186	C11H22O2	000112-37-8	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012417\
Data File : BF092458.D
Acq On : 25 Jan 2017 4:42
Operator : UM/SJ
Sample : I1397-04
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-12

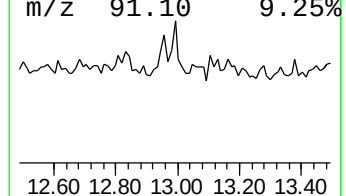
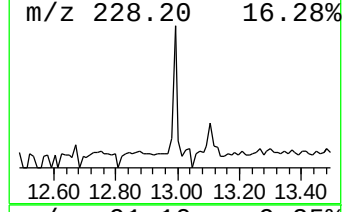
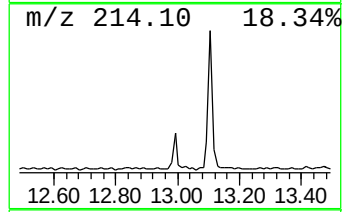
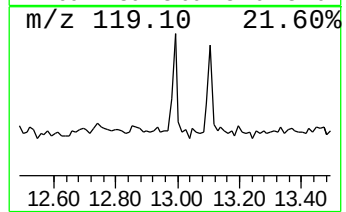
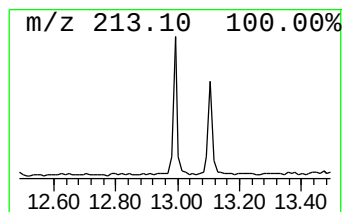
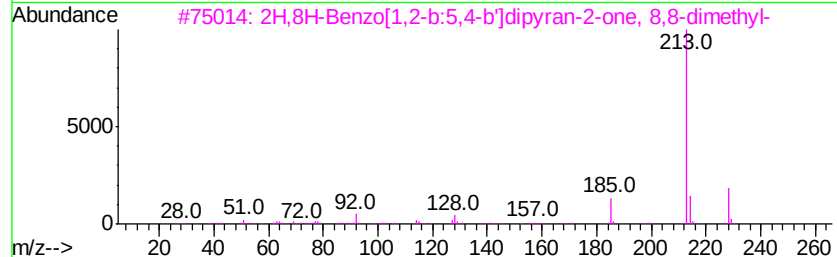
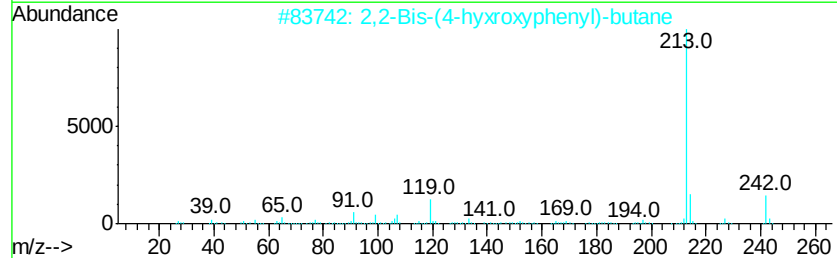
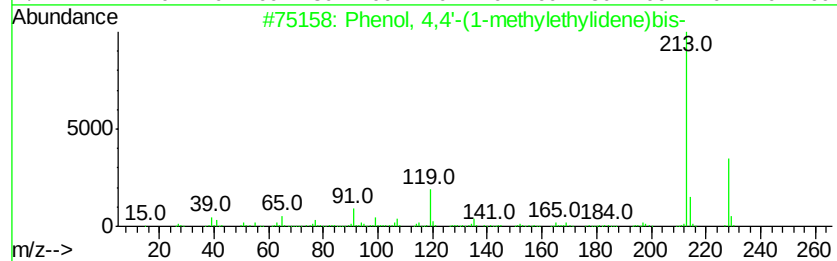
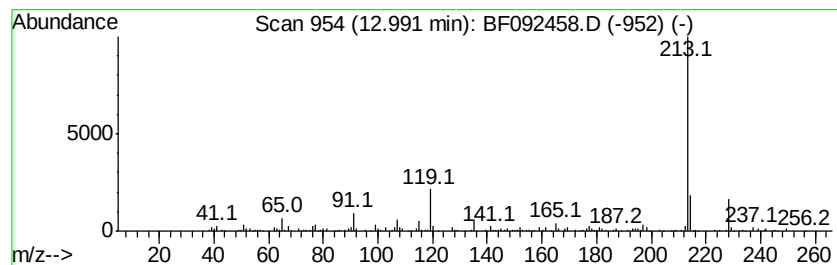
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phenol, 4,4'-(1-methylethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.99	2.05 ng	86726	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 4,4'-(1-methylethylidene)bis-	228	C15H16O2	000080-05-7	94
2		2,2-Bis-(4-hydroxyphenyl)-butane	242	C16H18O2	000077-40-7	59
3		2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	53
4		Pyridine, 3-(5-trifluoromethyl-3...	213	C9H6F3N3	003974-70-7	50
5		1,4-Puran, 5,6-dihydro-3-[3-indo...	213	C14H15NO	1000128-72-9	42



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012417\
Data File : BF092458.D
Acq On : 25 Jan 2017 4:42
Operator : UM/SJ
Sample : I1397-04
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-12

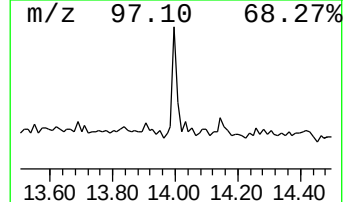
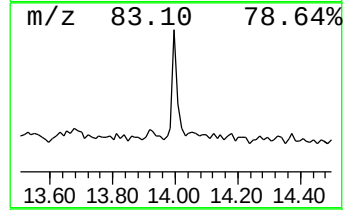
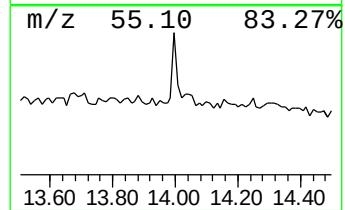
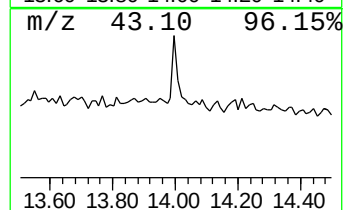
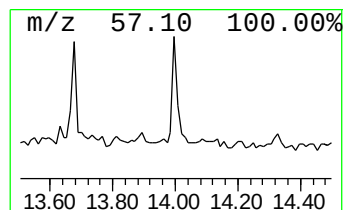
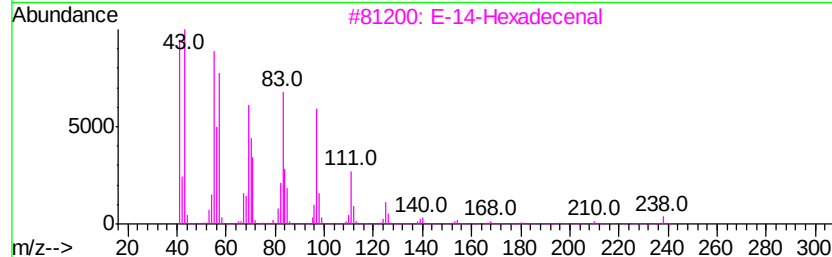
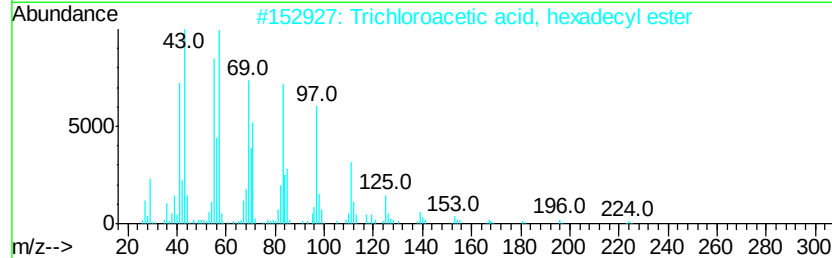
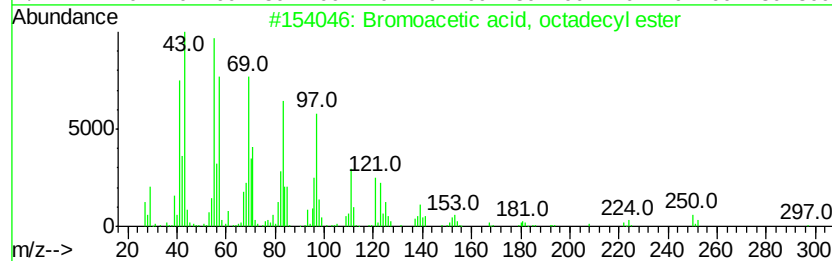
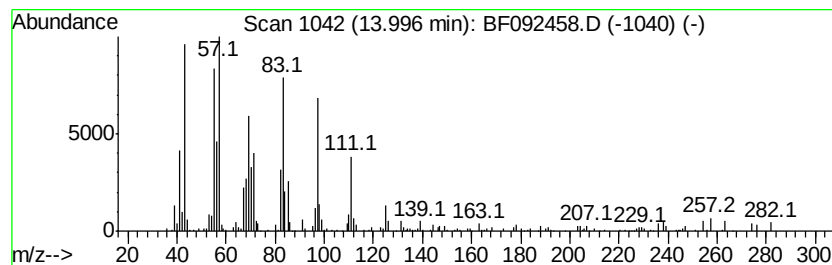
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Bromoacetic acid, octadecyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.00	2.04 ng	86387	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
3		E-14-Hexadecenal	238	C16H30O	330207-53-9	83
4		11-Tricosene	322	C23H46	052078-56-5	80
5		1-Docosene	308	C22H44	001599-67-3	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012417\
Data File : BF092458.D
Acq On : 25 Jan 2017 4:42
Operator : UM/SJ
Sample : I1397-04
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-12

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	11.4	ng	568896	1	6.97	1001420	20.0
unknown6.73	6.73	72.6	ng	3634250	1	6.97	1001420	20.0
Benzenesulfonamid...	10.69	54.5	ng	3749430	3	10.03	1376910	20.0
Benzenesulfonamid...	10.90	60.6	ng	3770610	4	11.52	1243610	20.0
Tridecanoic acid	12.04	3.7	ng	227418	4	11.52	1243610	20.0
Phenol, 4,4'-(1-m...	12.99	2.0	ng	86726	5	14.16	845174	20.0
Bromoacetic acid,...	14.00	2.0	ng	86387	5	14.16	845174	20.0