

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080416\
 Data File : BF089619.D
 Acq On : 5 Aug 2016 8:38
 Operator : UM/SJ
 Sample : H4288-25
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GW-66-6.5-15.0

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-BF080416.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	1.690	8	9	38	rVB	122457	428740	25.40%	3.685%
2	4.650	266	268	283	rBV	60699	132972	7.88%	1.143%
3	5.336	325	328	354	rBV	225831	583334	34.55%	5.014%
4	6.982	470	472	479	rBV	140516	366944	21.74%	3.154%
5	7.084	479	481	503	rVB	668012	1144556	67.80%	9.837%
6	7.450	511	513	523	rBV	107830	234799	13.91%	2.018%
7	7.587	523	525	530	rVV	23387	35548	2.11%	0.306%
8	7.679	530	533	550	rVV	760570	1021526	60.51%	8.780%
9	8.353	589	592	618	rBV	501425	800630	47.42%	6.881%
10	9.473	687	690	705	rBV	210777	362933	21.50%	3.119%
11	11.256	842	846	861	rBV	1095748	1688209	100.00%	14.510%
12	12.296	934	937	944	rBV	276555	432205	25.60%	3.715%
13	13.576	1047	1049	1060	rBV	517173	924427	54.76%	7.945%
14	13.919	1076	1079	1083	rBV	9276	17545	1.04%	0.151%
15	14.685	1144	1146	1154	rBV	292413	413702	24.51%	3.556%
16	15.702	1232	1235	1240	rBV	33742	60253	3.57%	0.518%
17	16.697	1316	1322	1329	rBV2	274972	652369	38.64%	5.607%
18	16.800	1329	1331	1339	rVB	52403	88937	5.27%	0.764%
19	16.914	1339	1341	1346	rVB2	19696	28506	1.69%	0.245%
20	17.051	1350	1353	1356	rBV	1042434	1465377	86.80%	12.595%
21	17.611	1400	1402	1406	rBV5	6877	17524	1.04%	0.151%
22	18.045	1438	1440	1446	rVB3	11268	25113	1.49%	0.216%
23	18.308	1461	1463	1468	rBV2	17173	34266	2.03%	0.295%
24	18.388	1468	1470	1474	rBV	212600	319700	18.94%	2.748%
25	18.846	1508	1510	1515	rVB2	11298	23895	1.42%	0.205%
26	19.086	1528	1531	1532	rBV3	9128	18075	1.07%	0.155%
27	19.223	1541	1543	1548	rVB2	13668	24543	1.45%	0.211%
28	19.588	1573	1575	1580	rVB3	10195	19397	1.15%	0.167%
29	20.046	1613	1615	1624	rVB	188038	245040	14.51%	2.106%
30	20.903	1687	1690	1698	rVB5	8391	23803	1.41%	0.205%

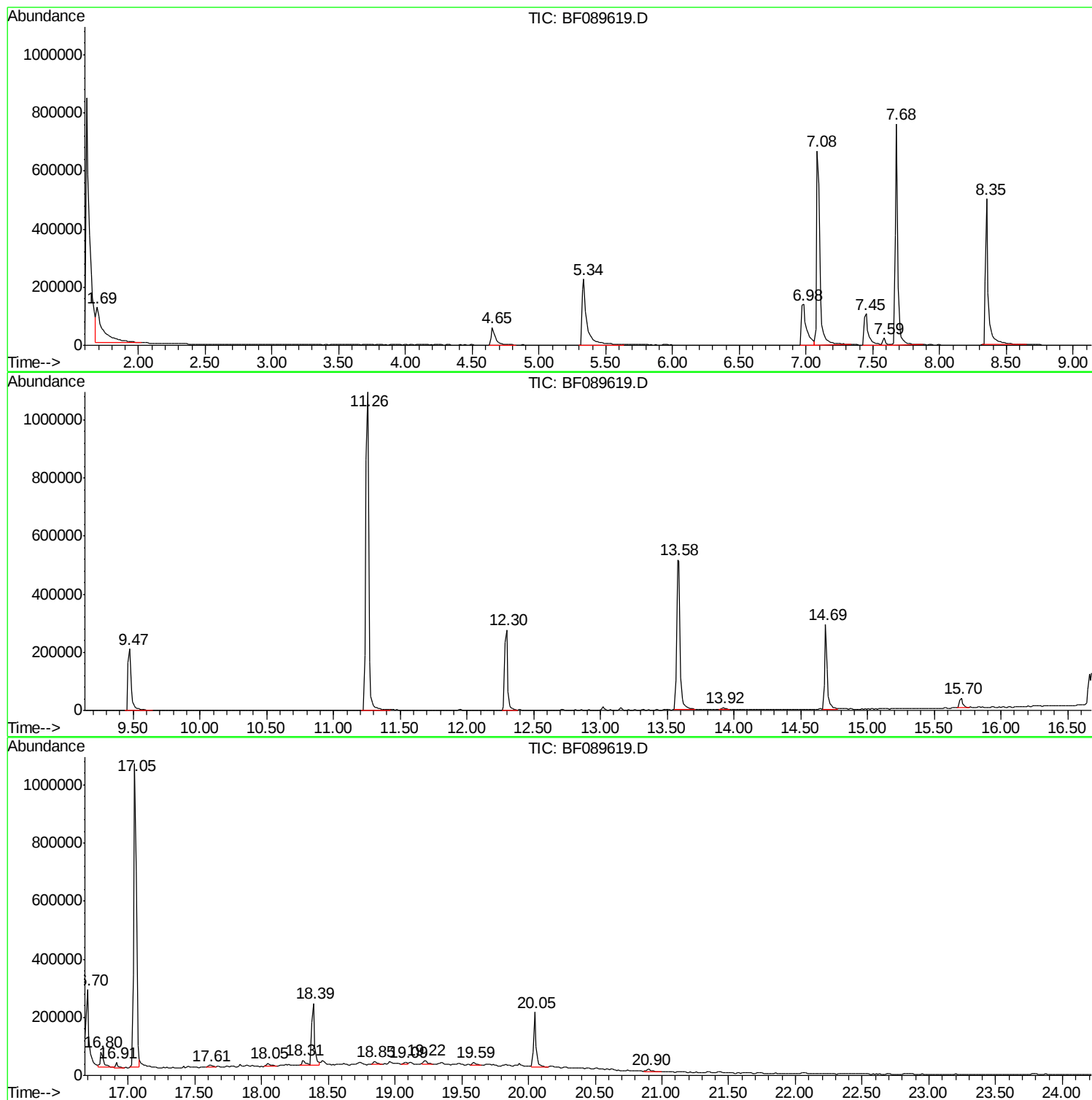
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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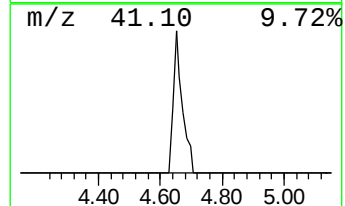
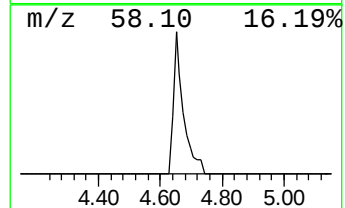
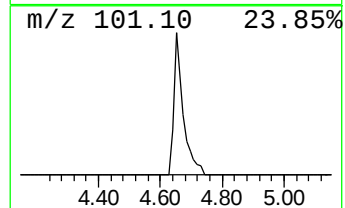
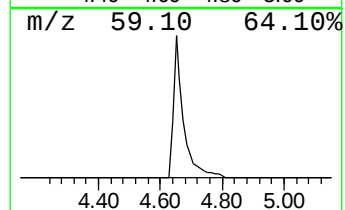
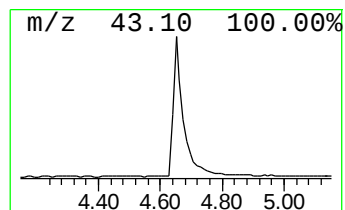
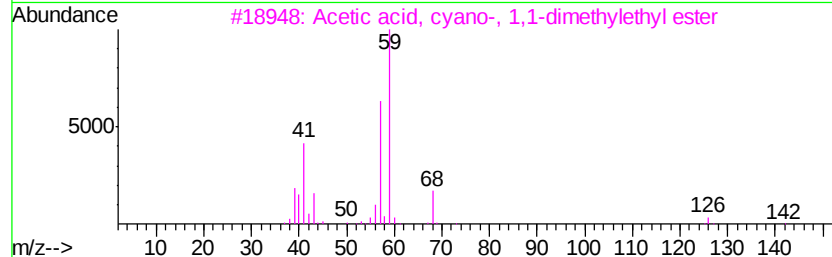
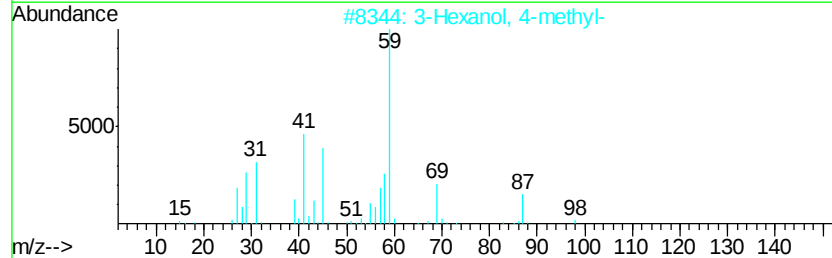
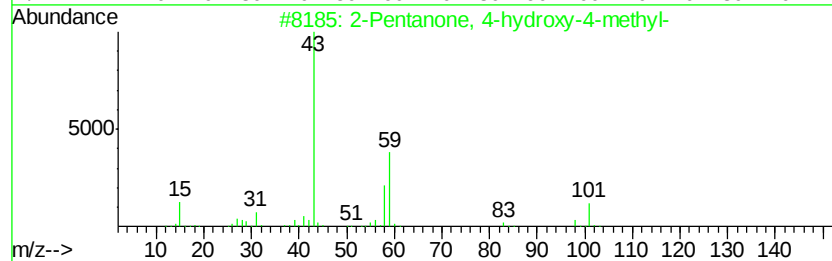
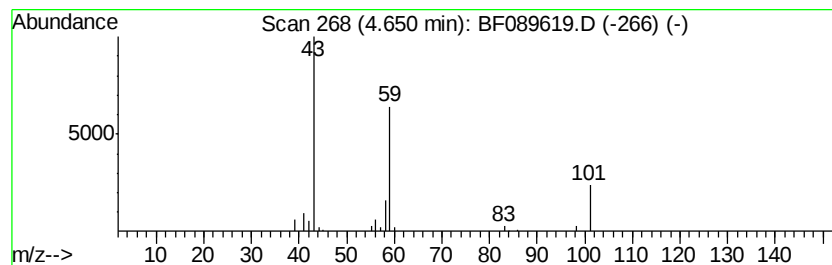
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.65	11.33 ng	132972	1,4-Dichlorobenzene-d4	7.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Acetone	58	C3H6O	000067-64-1	9



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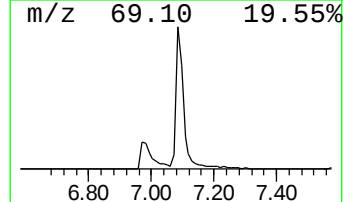
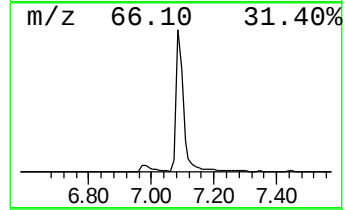
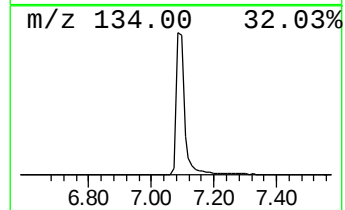
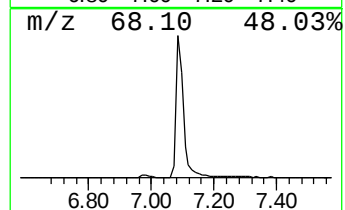
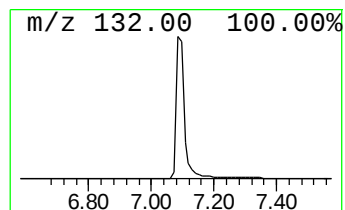
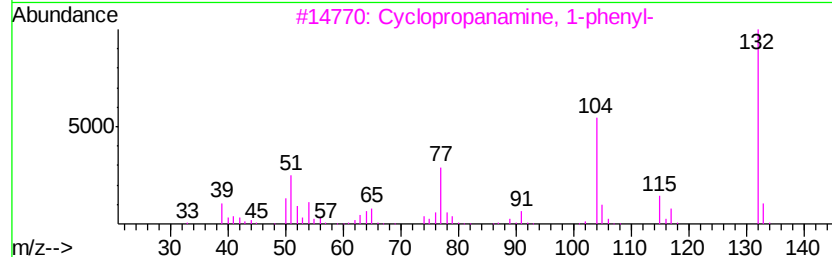
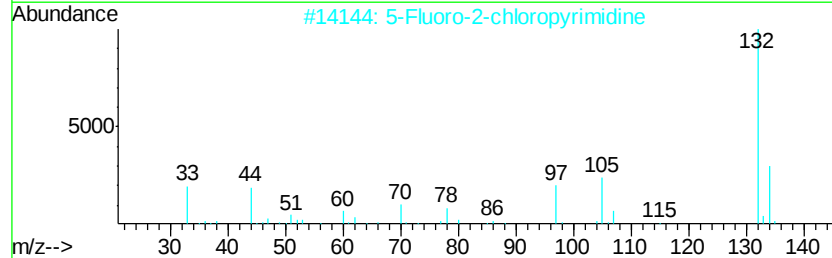
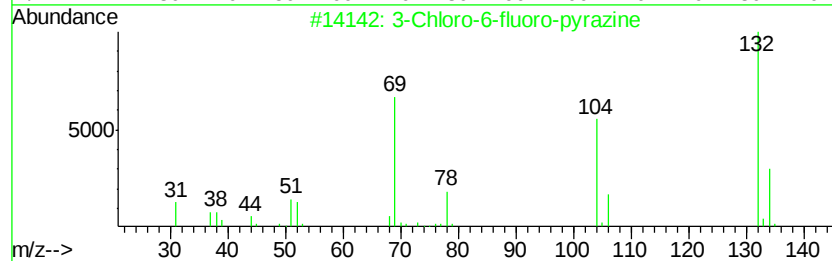
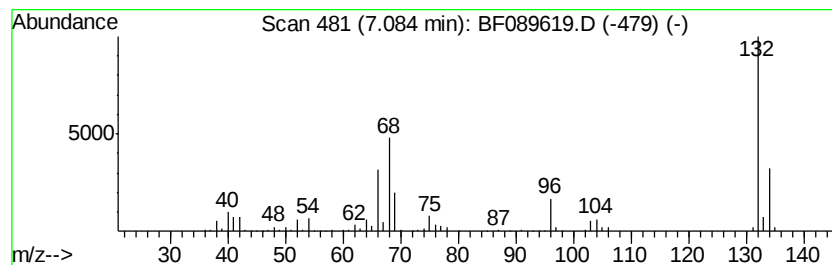
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Peak Number 3 unknown7.08 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.08	97.49 ng	1144560	1,4-Dichlorobenzene-d4	7.45

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		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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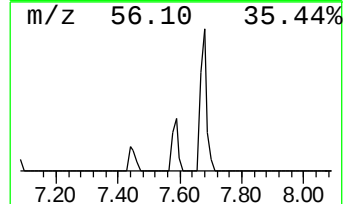
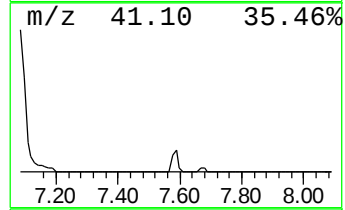
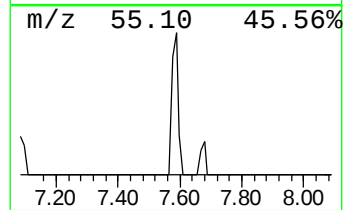
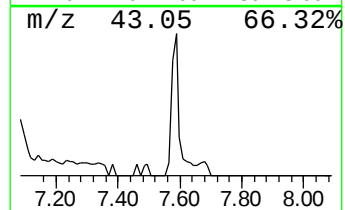
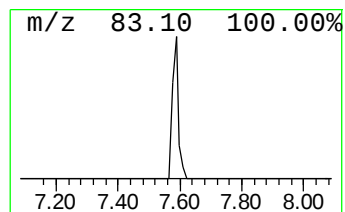
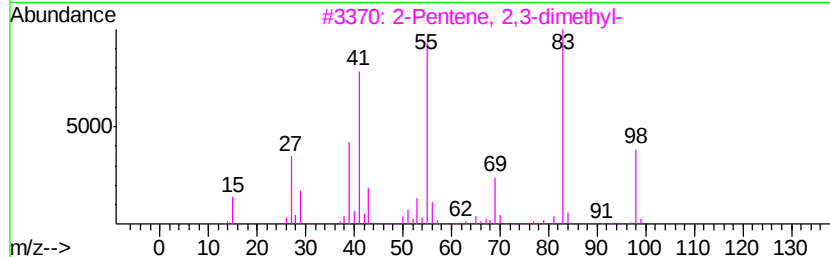
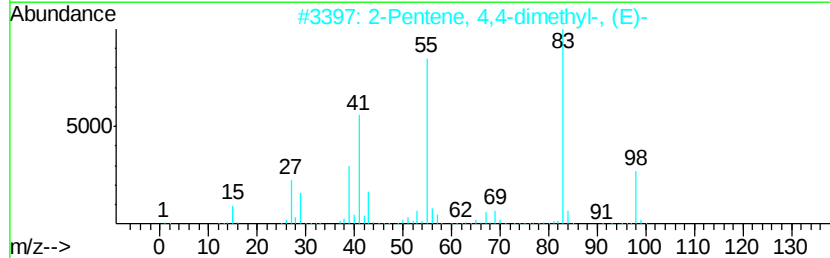
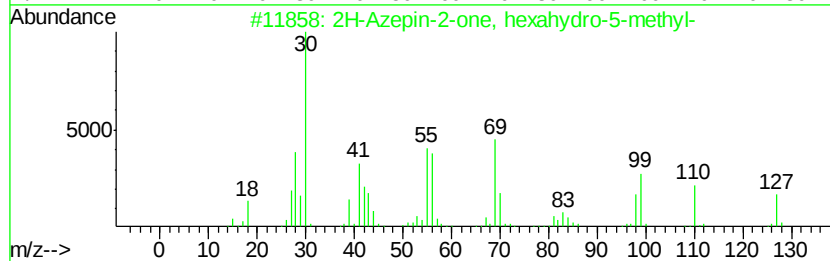
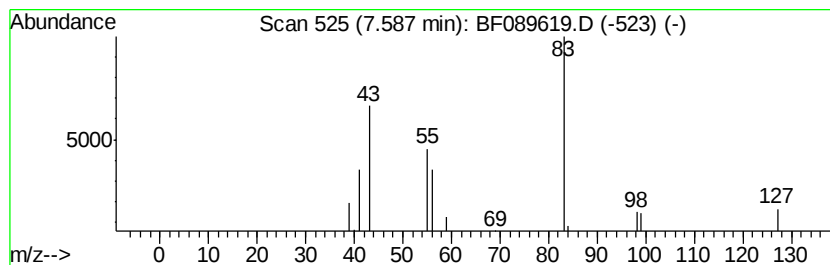
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 unknown7.59 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	3.03 ng	35548	1,4-Dichlorobenzene-d4	7.45

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-Azepin-2-one, hexahydro-5-met...	127	C7H13NO	002210-07-3	22
2			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	9
3			2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	9
4			1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	9
5			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	9



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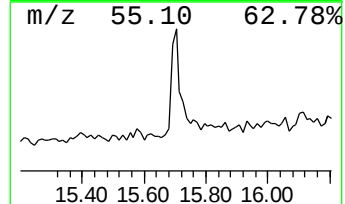
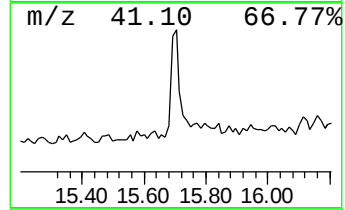
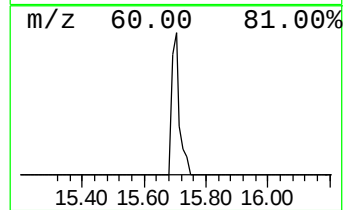
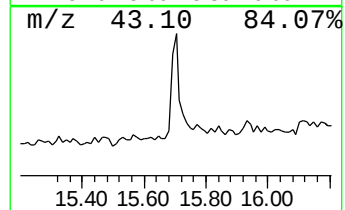
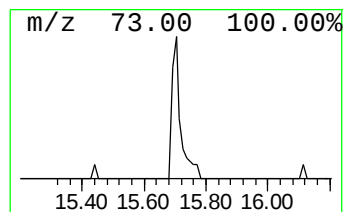
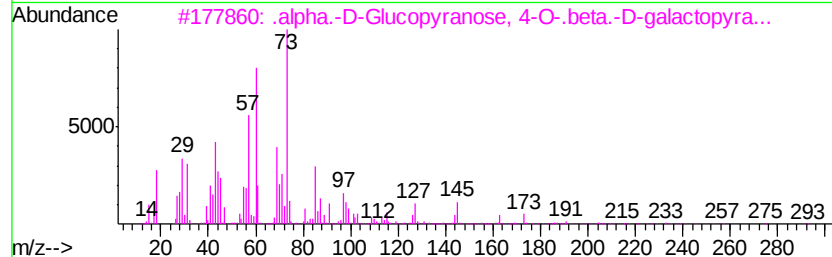
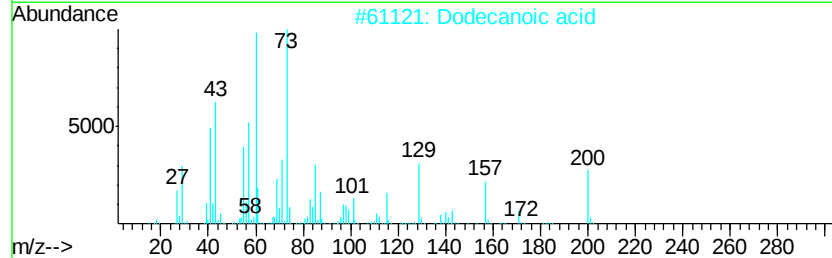
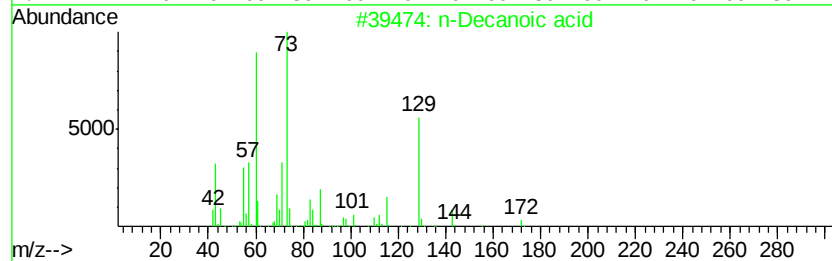
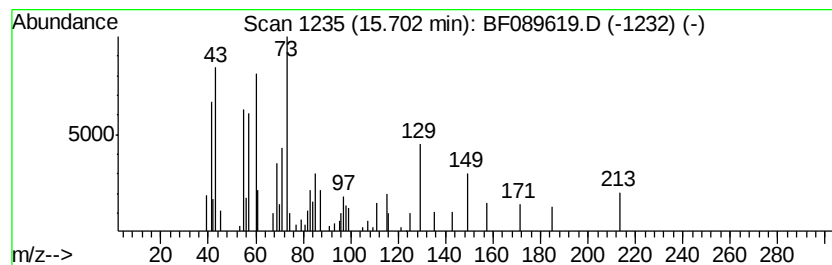
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Peak Number 6 n-Decanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	2.91 ng	60253	Phenanthrene-d10	14.69

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Decanoic acid	172	C10H20O2	000334-48-5	53
2		Dodecanoic acid	200	C12H24O2	000143-07-7	50
3		.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	22
4		1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	11
5		1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	11



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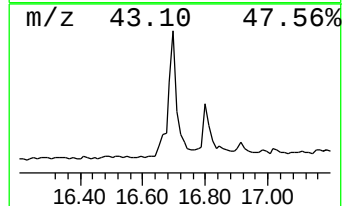
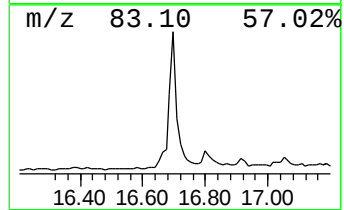
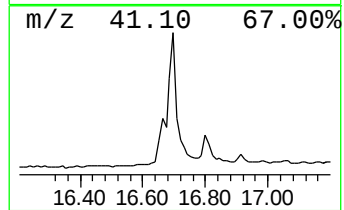
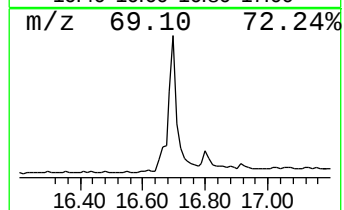
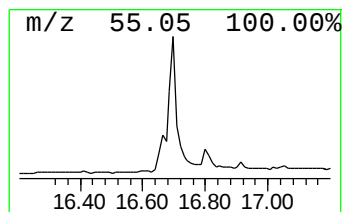
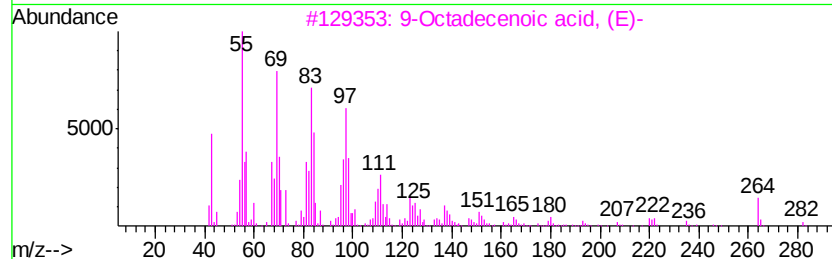
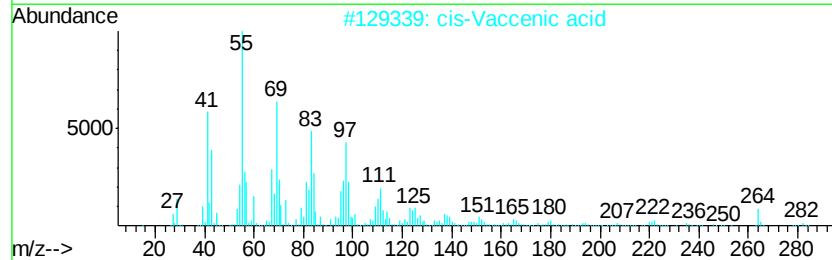
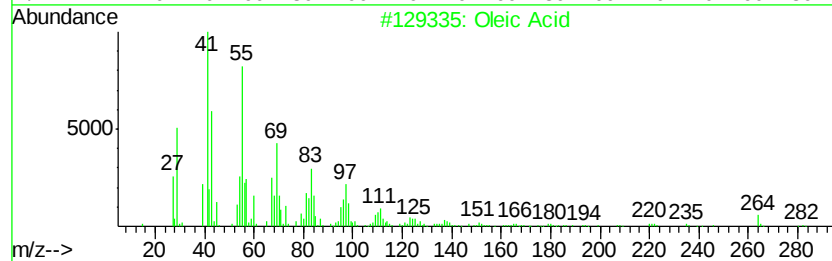
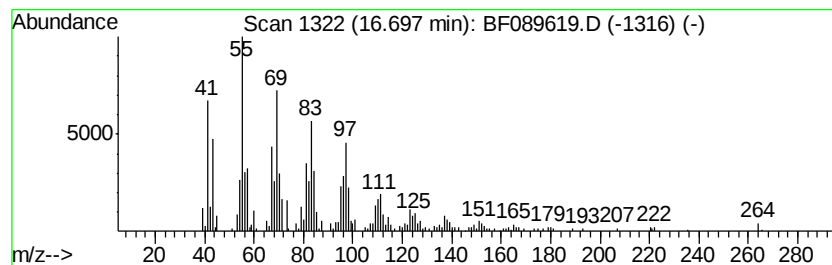
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Peak Number 7 Oleic Acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
16.70	40.81 ng	652369	Chrysene-d12		18.39
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oleic Acid	282	C18H34O2	000112-80-1	91
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	90
3	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	76
4	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	72
5	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	70



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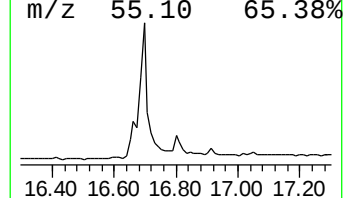
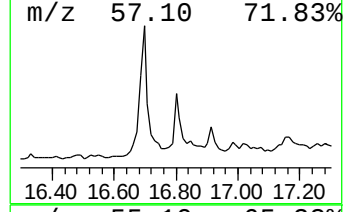
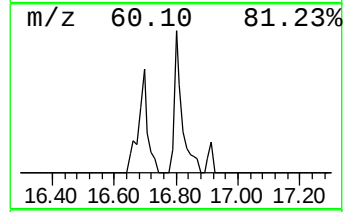
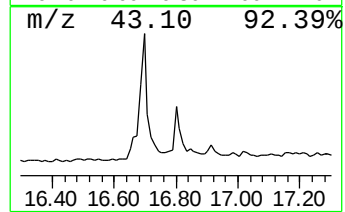
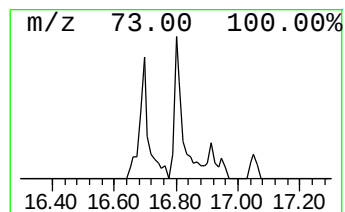
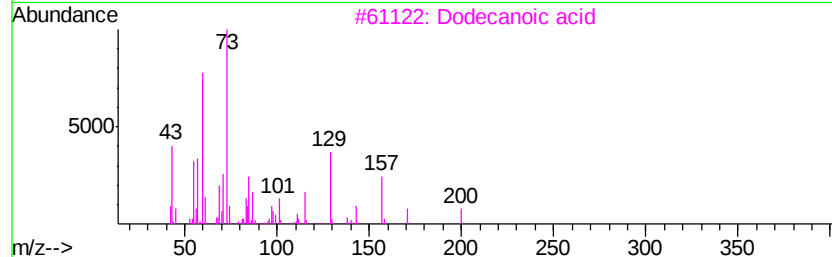
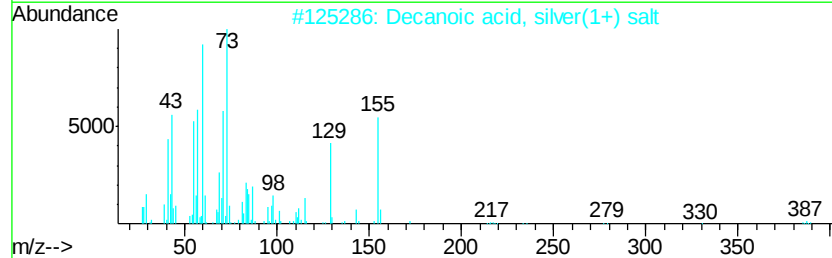
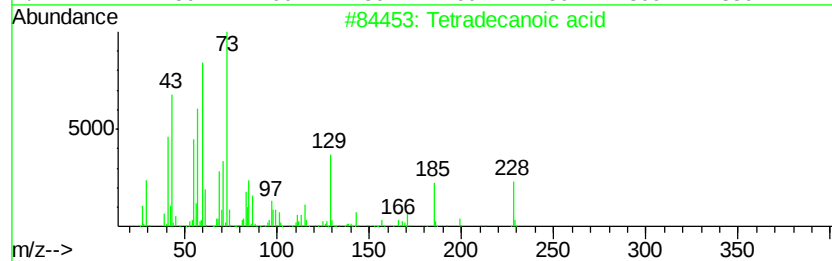
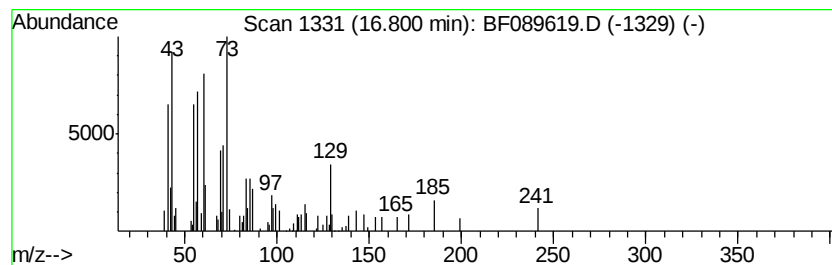
Instrument :
BNA_F
ClientSampleId :
GW-66-6.5-15.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.80	5.56 ng	88937	Chrysene-d12	18.39	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
2	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64
3	Dodecanoic acid	200	C12H24O2	000143-07-7	59
4	Undecanoic acid	186	C11H22O2	000112-37-8	43
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080416\
Data File : BF089619.D
Acq On : 5 Aug 2016 8:38
Operator : UM/SJ
Sample : H4288-25
Misc :
ALS Vial : 27 Sample Multiplier: 1

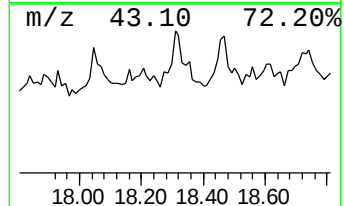
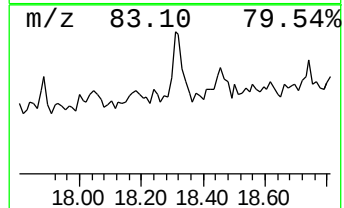
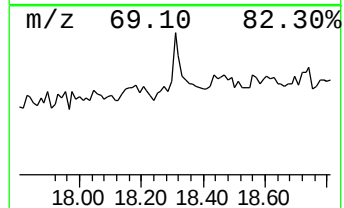
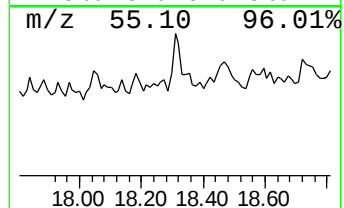
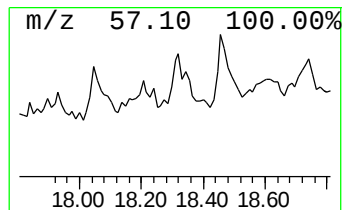
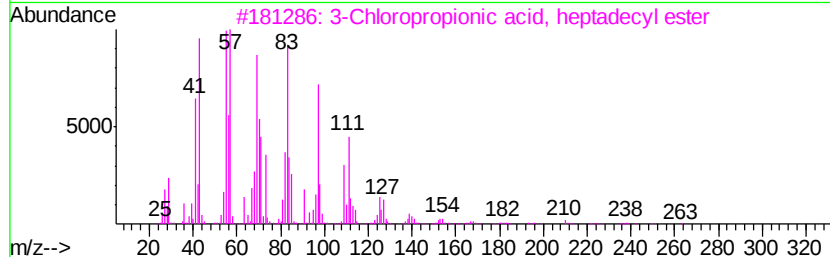
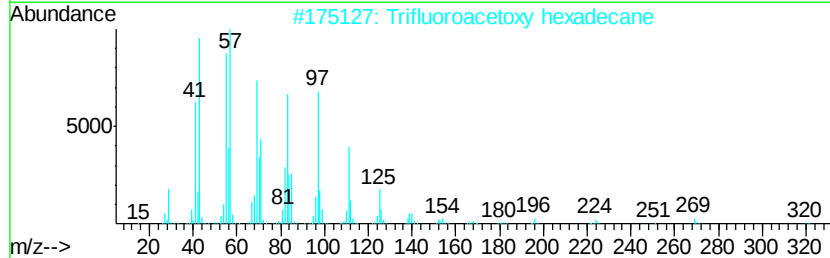
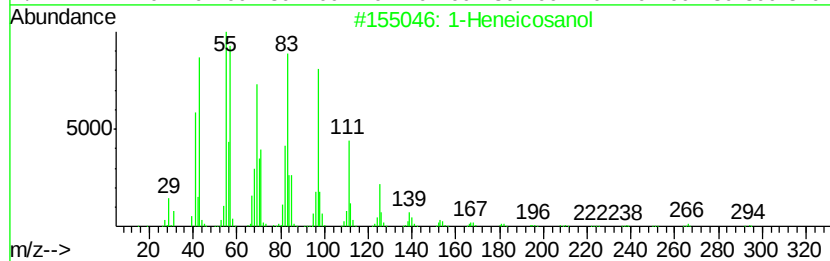
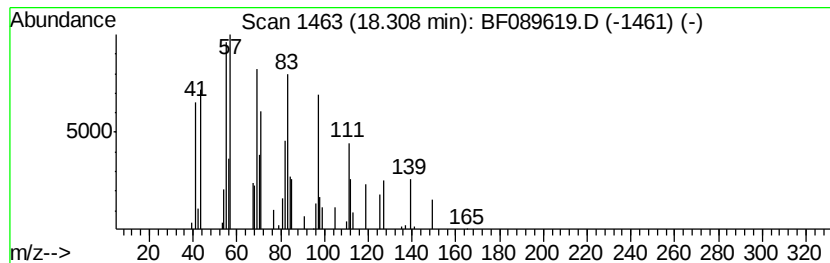
Instrument :
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ClientSampleId :
GW-66-6.5-15.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heneicosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.31	2.14 ng	34266	Chrysene-d12	18.39
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heneicosanol	312 C21H44O	015594-90-8	81
2	Trifluoroacetoxy hexadecane	338 C18H33F3O2	006222-03-3	81
3	3-Chloropropionic acid, heptadec...	346 C20H39ClO2	1000283-05-1	72
4	Trichloroacetic acid, pentadecyl...	372 C17H31Cl3O2	074339-53-0	68
5	Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080416\
Data File : BF089619.D
Acq On : 5 Aug 2016 8:38
Operator : UM/SJ
Sample : H4288-25
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-66-6.5-15.0

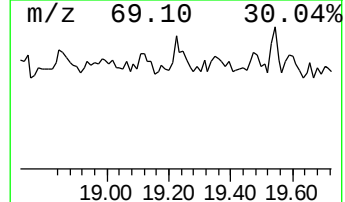
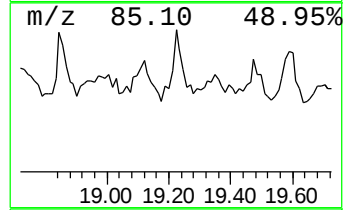
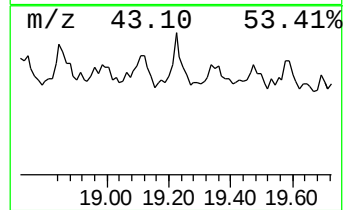
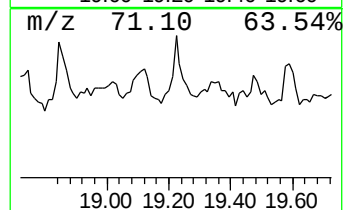
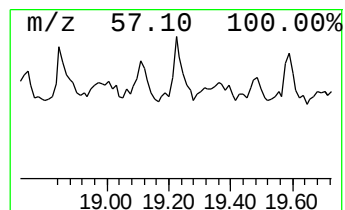
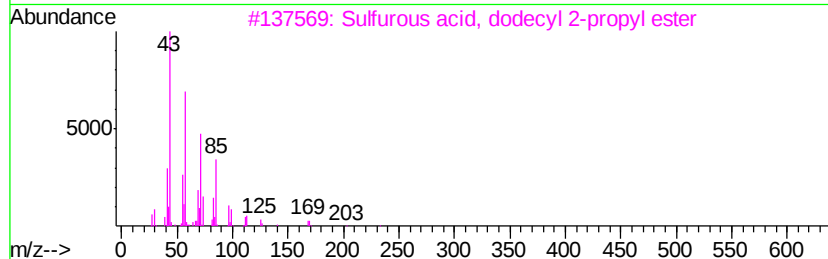
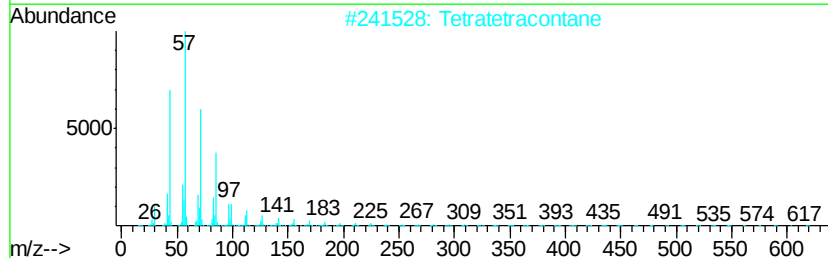
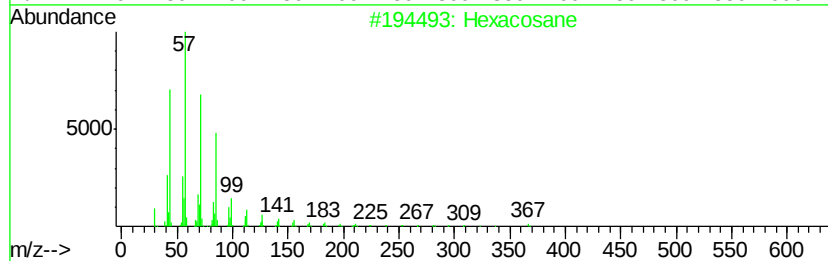
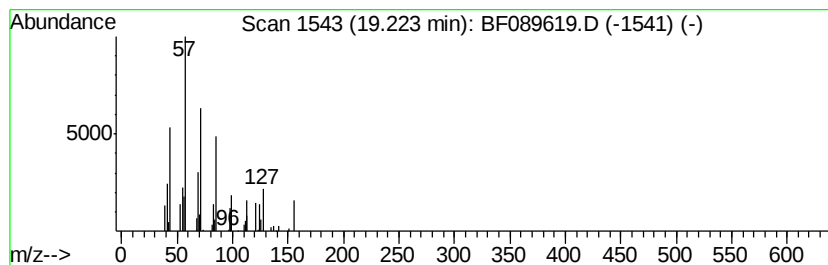
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.22	2.00 ng	24543	Perylene-d12	20.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	53
2		Tetratetracontane	619	C44H90	007098-22-8	53
3		Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	50
4		10-Methylnonadecane	282	C20H42	056862-62-5	50
5		Hexadecane	226	C16H34	000544-76-3	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080416\
Data File : BF089619.D
Acq On : 5 Aug 2016 8:38
Operator : UM/SJ
Sample : H4288-25
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-66-6.5-15.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.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...	4.65	11.3	ng	132972	1	7.45	234799	20.0
unknown7.08	7.08	97.5	ng	1144560	1	7.45	234799	20.0
unknown7.59	7.59	3.0	ng	35548	1	7.45	234799	20.0
n-Decanoic acid	15.70	2.9	ng	60253	4	14.69	413702	20.0
Oleic Acid	16.70	40.8	ng	652369	5	18.39	319700	20.0
Tetradecanoic acid	16.80	5.6	ng	88937	5	18.39	319700	20.0
1-Heneicosanol	18.31	2.1	ng	34266	5	18.39	319700	20.0
Hexacosane	19.22	2.0	ng	24543	6	20.05	245040	20.0