

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080217\
 Data File : BF097276.D
 Acq On : 2 Aug 2017 16:34
 Operator : SJ/JU
 Sample : I4497-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1

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-BF072517.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	2.604	119	122	139	rBV	183163	405498	15.15%	1.647%
2	4.581	454	458	468	rBV	284535	463237	17.31%	1.882%
3	5.051	534	538	556	rBV	2239737	2474556	92.48%	10.052%
4	6.122	716	720	733	rBV	2481219	2675778	100.00%	10.869%
5	6.222	733	737	755	rVB	2494578	2459408	91.91%	9.990%
6	6.451	772	776	783	rBV	701638	683215	25.53%	2.775%
7	6.604	798	802	811	rBV	1925697	1712007	63.98%	6.954%
8	7.016	868	872	887	rBV	1361743	1447403	54.09%	5.879%
9	7.163	894	897	905	rVV	32808	40071	1.50%	0.163%
10	7.257	909	913	916	rBV	32306	30597	1.14%	0.124%
11	7.663	979	982	990	rBV	85000	110782	4.14%	0.450%
12	7.733	990	994	1003	rVB	1080391	952440	35.59%	3.869%
13	8.810	1172	1177	1180	rBV	2376741	2233822	83.48%	9.074%
14	9.210	1241	1245	1250	rBV	653009	522812	19.54%	2.124%
15	9.474	1286	1290	1294	rBV2	1022503	883880	33.03%	3.590%
16	9.933	1365	1368	1371	rVB	36317	30220	1.13%	0.123%
17	10.021	1381	1383	1388	rVB	33535	28214	1.05%	0.115%
18	10.263	1420	1424	1436	rBV	1450043	1362006	50.90%	5.533%
19	10.398	1444	1447	1454	rBV	57491	71363	2.67%	0.290%
20	10.845	1518	1523	1526	rBV2	48165	42429	1.59%	0.172%
21	10.951	1537	1541	1543	rBV	907412	890543	33.28%	3.617%
22	10.968	1543	1544	1549	rVB	215273	174251	6.51%	0.708%
23	11.027	1549	1554	1558	rBV	69178	67878	2.54%	0.276%
24	11.504	1633	1635	1642	rVV2	118254	133364	4.98%	0.542%
25	11.557	1642	1644	1647	rBV	51794	44585	1.67%	0.181%
26	12.151	1741	1745	1749	rBV	304553	253910	9.49%	1.031%
27	12.286	1764	1768	1779	rBV2	73289	89206	3.33%	0.362%
28	12.374	1779	1783	1787	rBV	274438	267051	9.98%	1.085%
29	12.533	1805	1810	1813	rVB	1915608	1907066	71.27%	7.747%
30	12.709	1837	1840	1846	rVB	40987	40669	1.52%	0.165%
31	12.774	1848	1851	1854	rBV	46649	41342	1.55%	0.168%
32	13.451	1961	1966	1977	rBV3	73035	130302	4.87%	0.529%
33	13.568	1979	1986	1989	rBV	853217	861383	32.19%	3.499%
34	13.592	1989	1990	1995	rVB	77771	68568	2.56%	0.279%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.333	2113	2116	2119	rBV	34321	33110	1.24%	0.134%
36	14.562	2151	2155	2158	rBV	60971	80337	3.00%	0.326%
37	14.651	2164	2170	2174	rBV5	26153	39136	1.46%	0.159%
38	14.809	2194	2197	2202	rVB2	34679	36550	1.37%	0.148%
39	14.862	2202	2206	2210	rBV	56521	59063	2.21%	0.240%
40	14.909	2210	2214	2219	rVV	441562	492616	18.41%	2.001%
41	14.956	2220	2222	2226	rVB	33131	30657	1.15%	0.125%
42	15.309	2277	2282	2286	rBV2	33986	49849	1.86%	0.202%
43	15.380	2291	2294	2302	rVB8	11212	27513	1.03%	0.112%
44	15.709	2345	2350	2359	rBV2	31543	61851	2.31%	0.251%
45	16.127	2416	2421	2425	rBV3	18276	31164	1.16%	0.127%
46	16.180	2425	2430	2436	rVB3	27994	45224	1.69%	0.184%
47	16.727	2519	2523	2528	rVB8	17313	31273	1.17%	0.127%

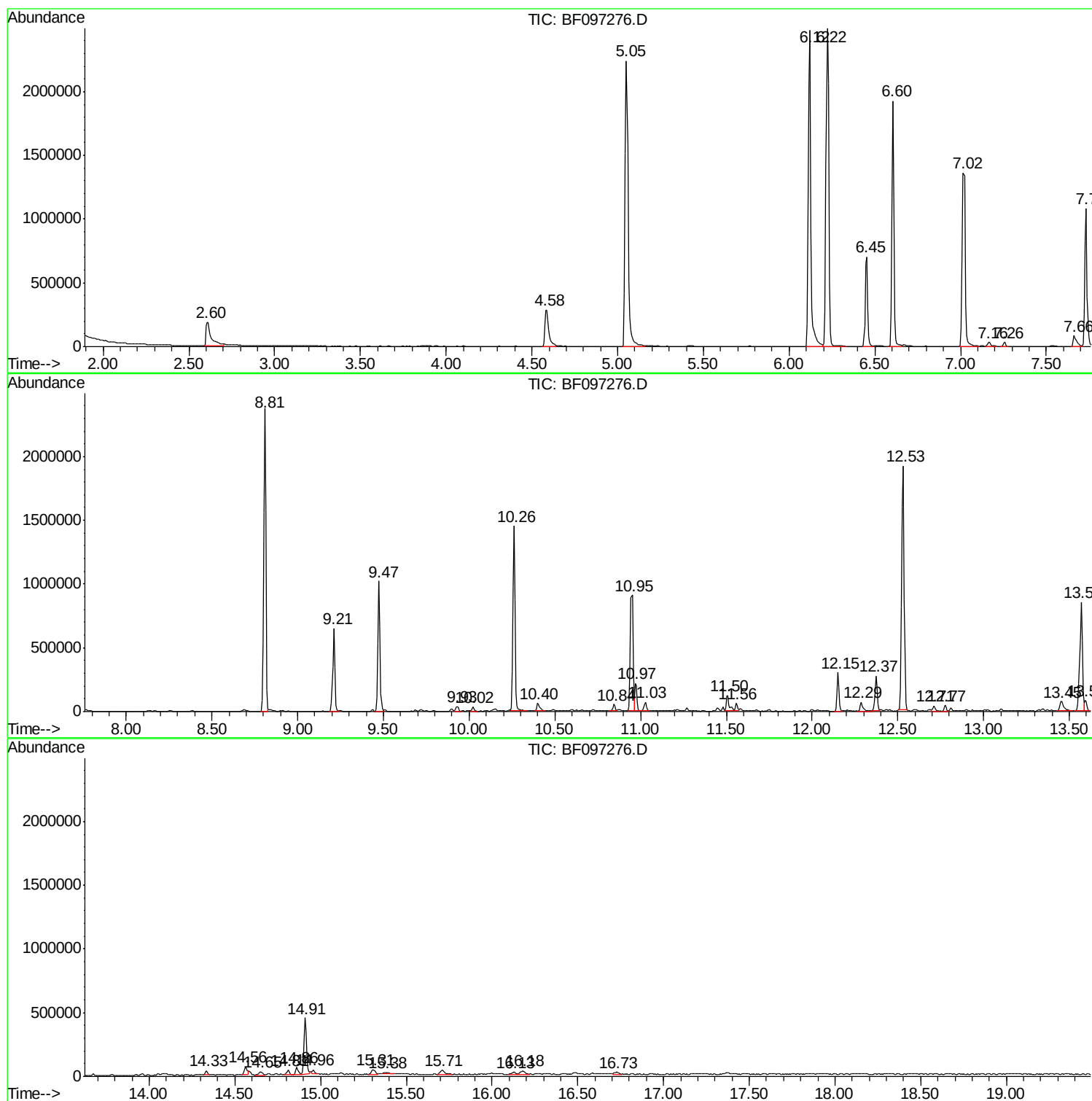
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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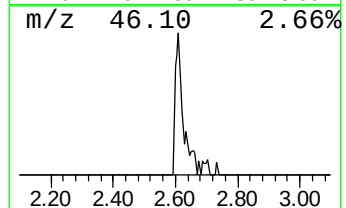
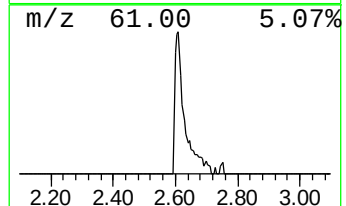
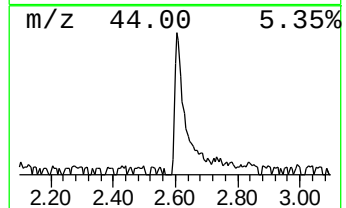
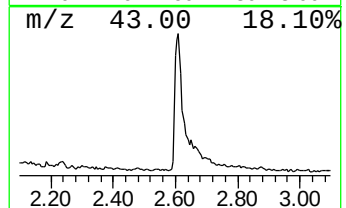
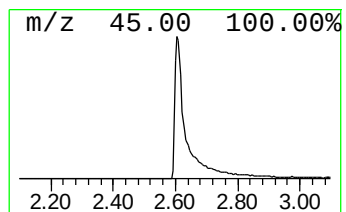
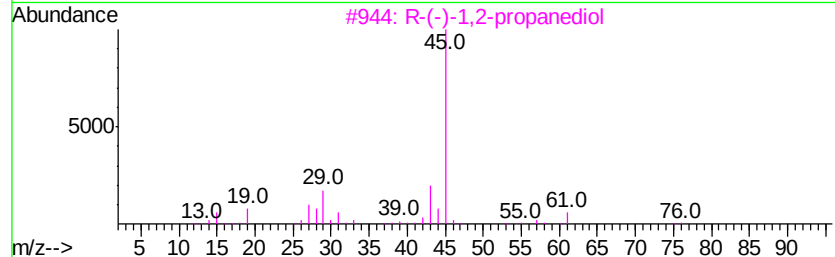
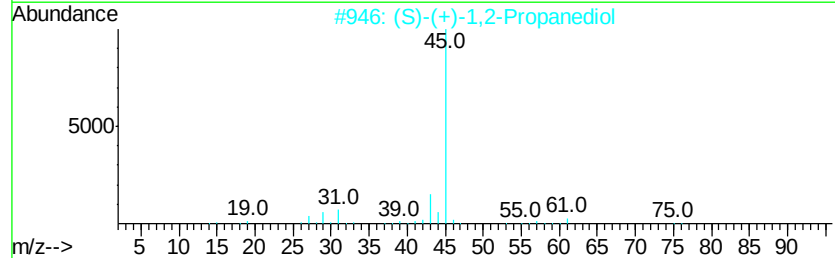
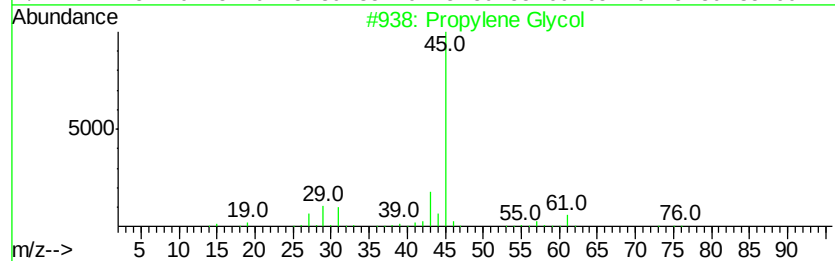
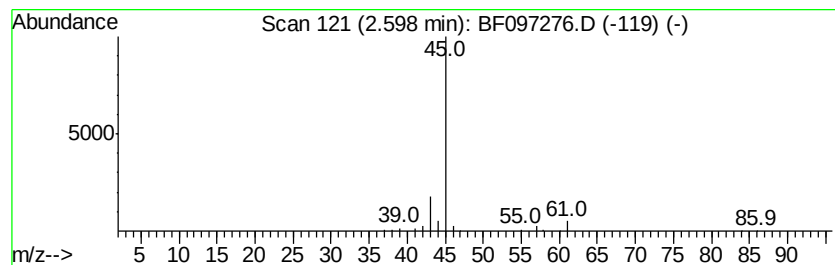
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.60	11.87 ng	405498	1,4-Dichlorobenzene-d4	6.45

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propylene Glycol	76	C3H8O2	000057-55-6	74
2		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
4		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9



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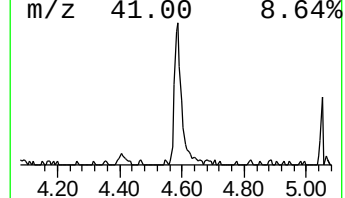
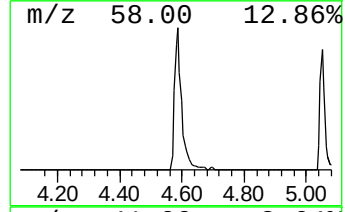
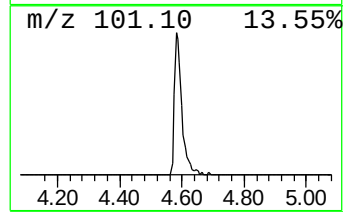
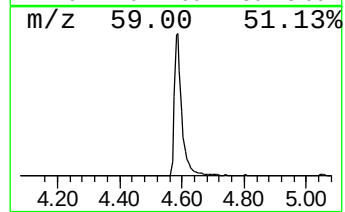
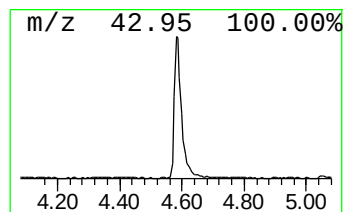
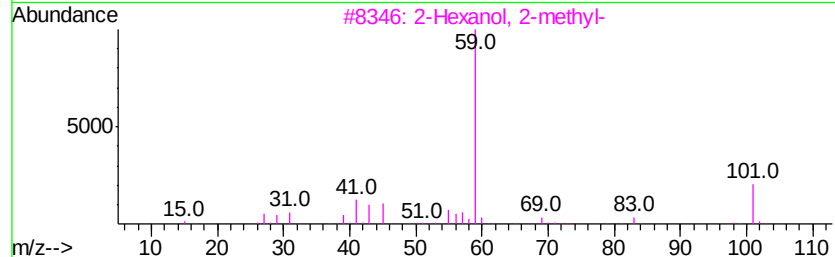
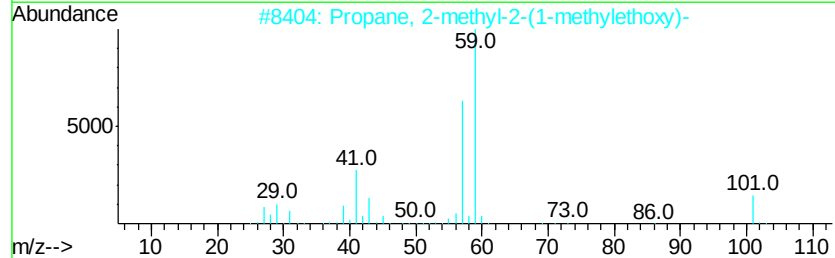
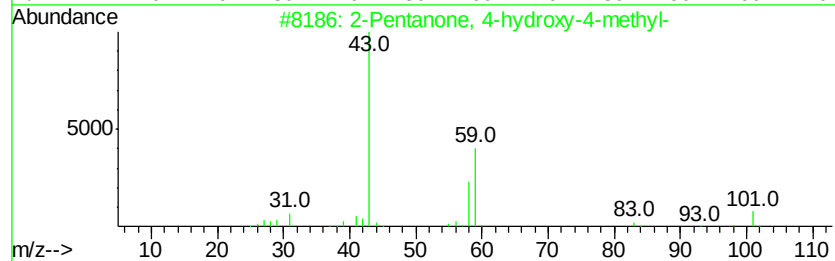
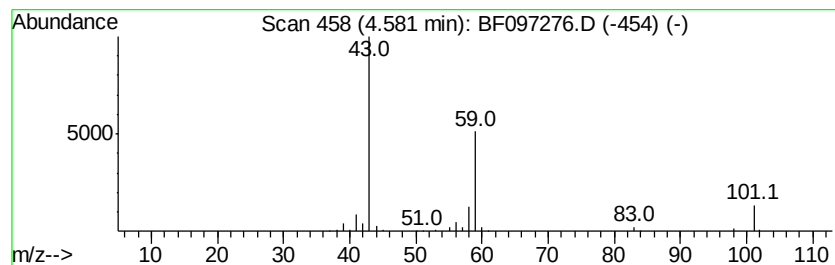
Instrument :
BNA_F
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TP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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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.		
4.58	13.56 ng	463237	1,4-Dichlorobenzene-d4	6.45		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33	
4	3-Hexanol	102	C6H14O	000623-37-0	33	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	



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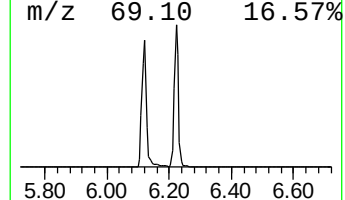
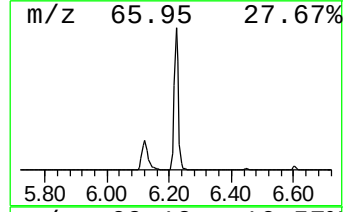
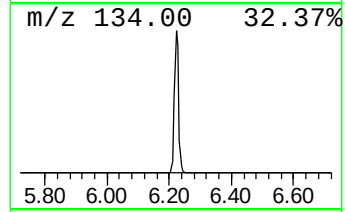
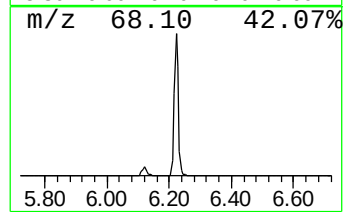
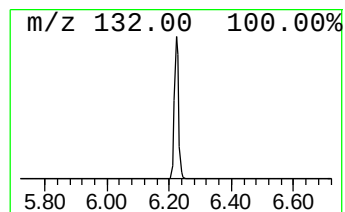
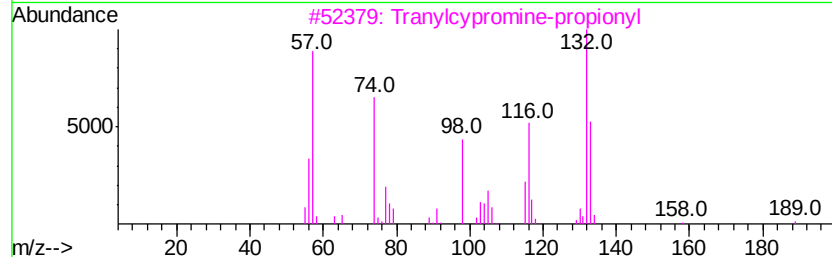
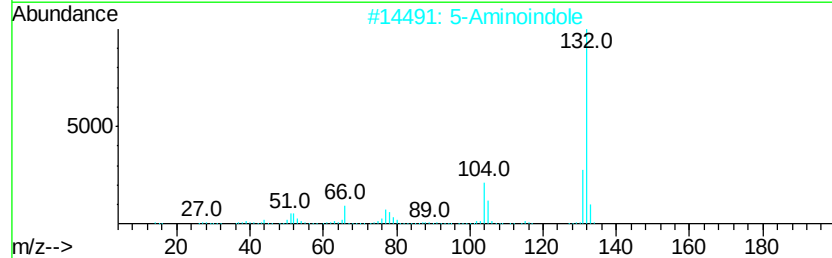
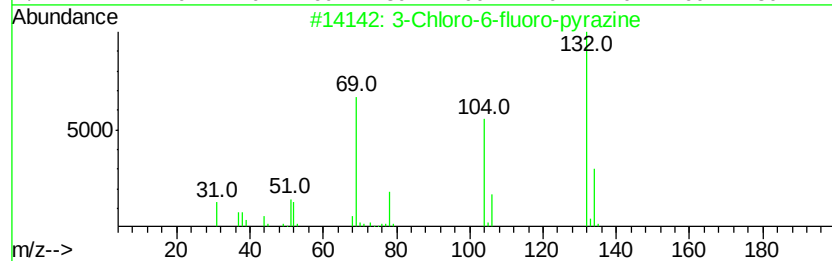
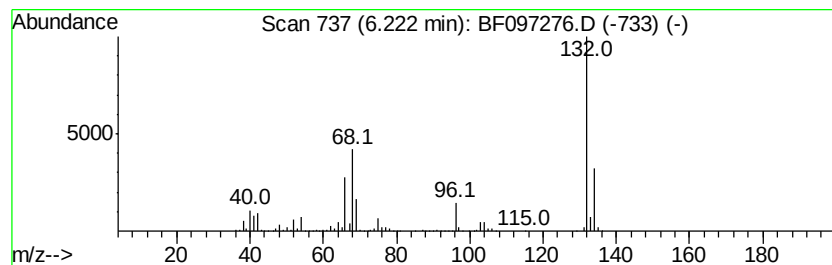
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.22 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.22	72.00 ng	2459410	1,4-Dichlorobenzene-d4	6.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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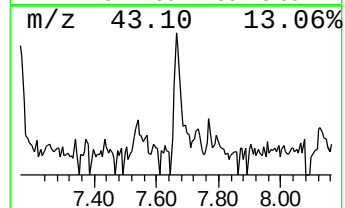
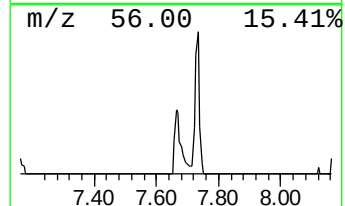
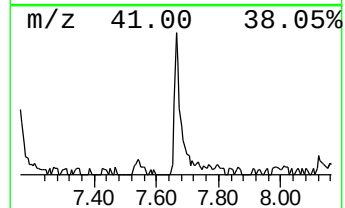
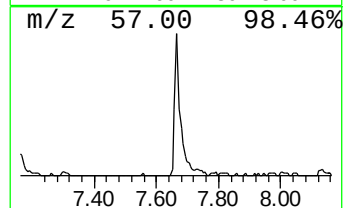
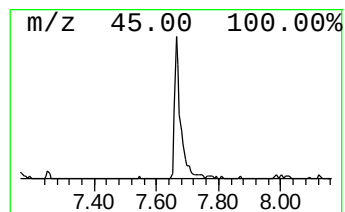
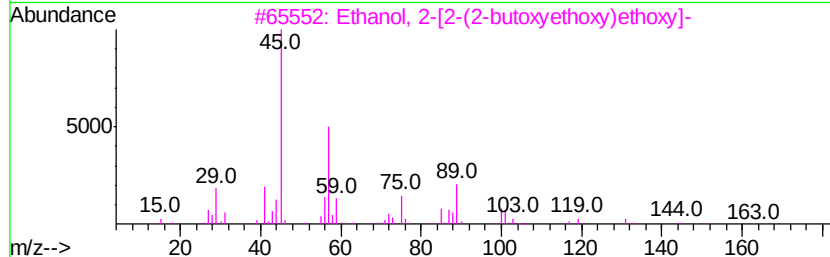
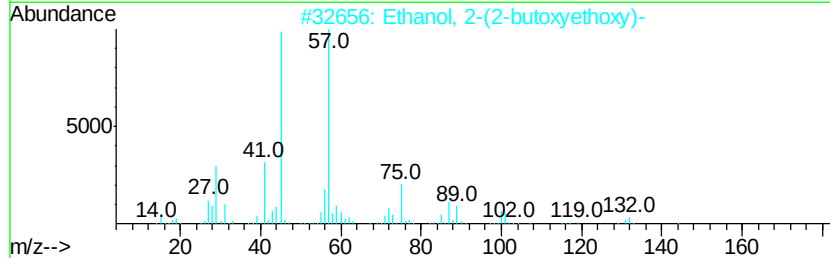
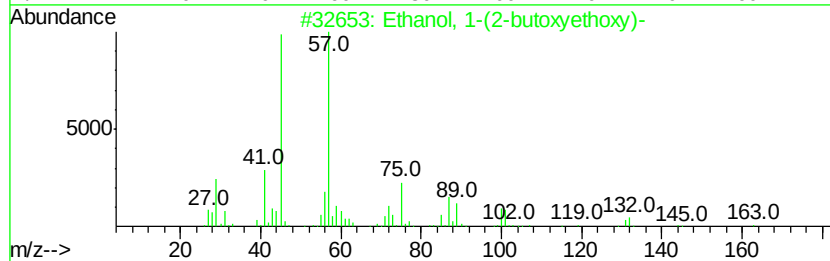
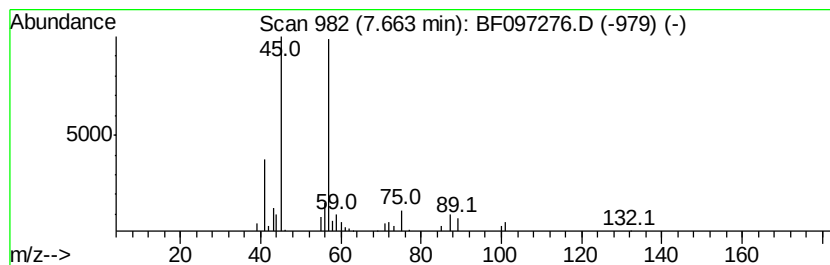
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	2.33 ng	110782	Naphthalene-d8	7.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	86
2		Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
3		Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	64
4		Tetraethylene glycol	194	C8H18O5	000112-60-7	59
5		Pentaethylene glycol	238	C10H22O6	004792-15-8	50



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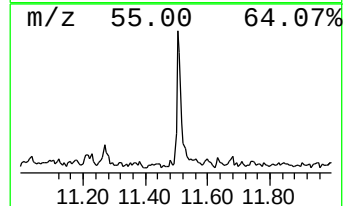
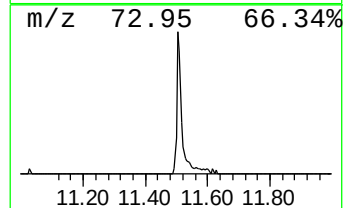
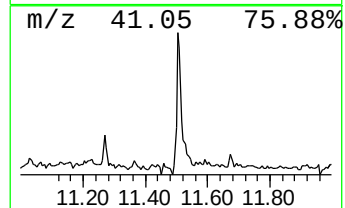
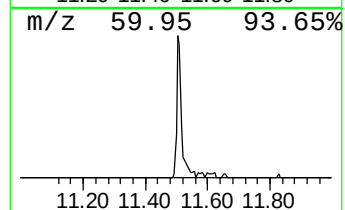
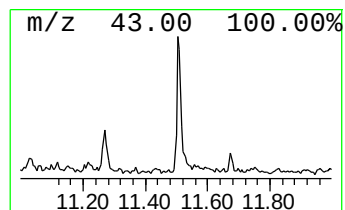
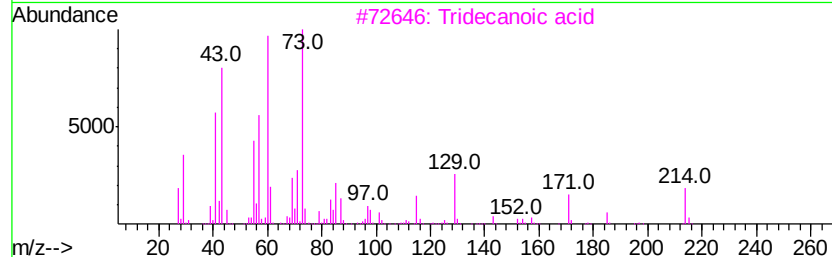
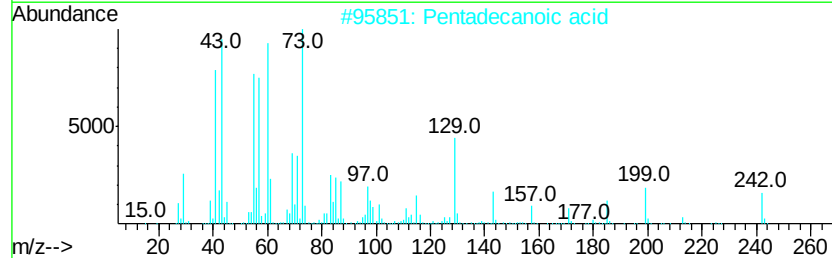
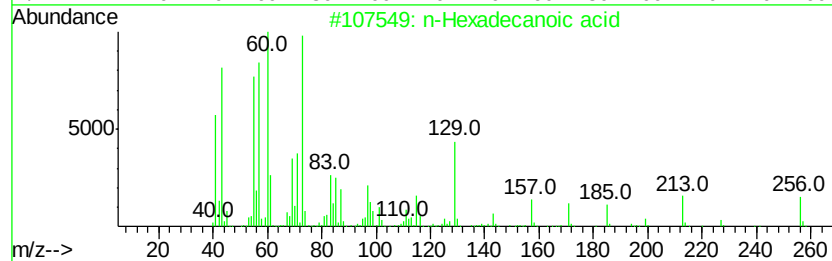
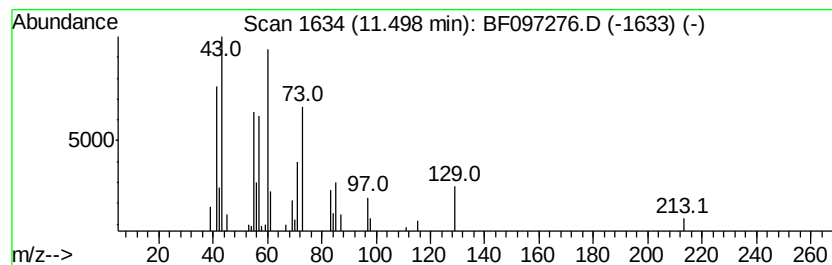
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.50	3.00 ng	133364	Phenanthrene-d10	10.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080217\
Data File : BF097276.D
Acq On : 2 Aug 2017 16:34
Operator : SJ/JU
Sample : I4497-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

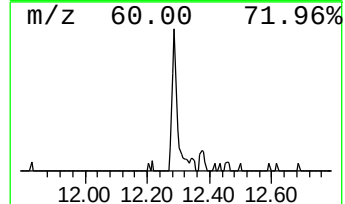
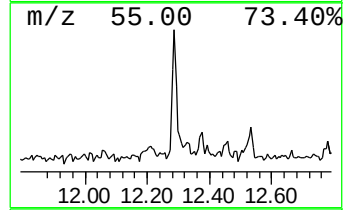
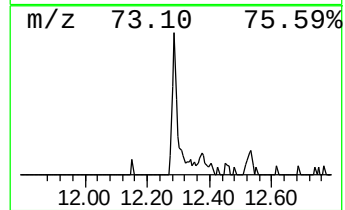
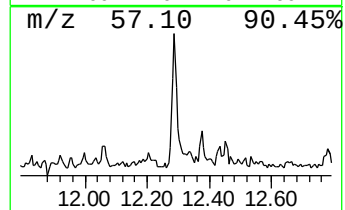
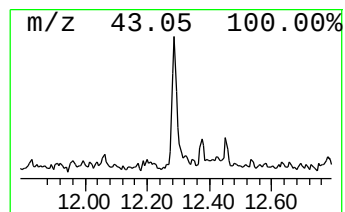
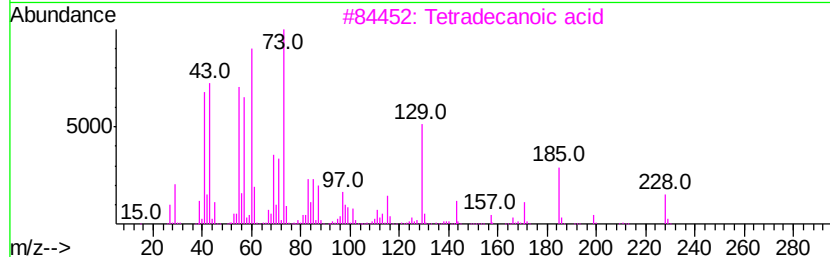
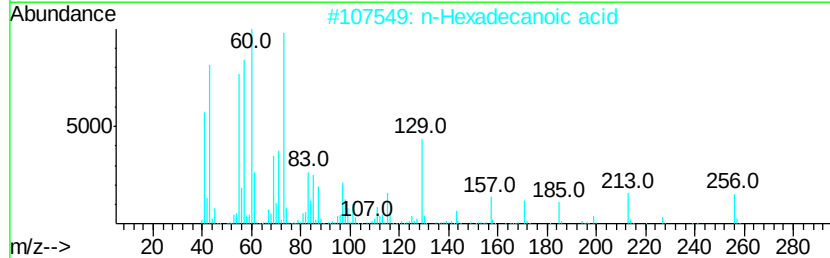
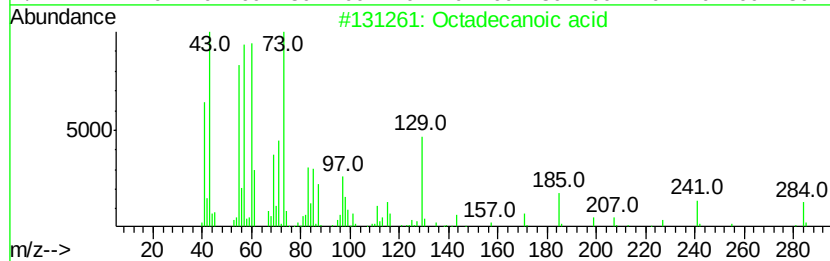
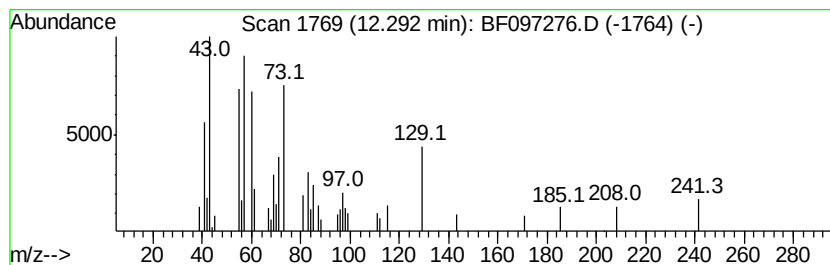
Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.29	2.07 ng	89206	Chrysene-d12		13.57
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080217\
Data File : BF097276.D
Acq On : 2 Aug 2017 16:34
Operator : SJ/JU
Sample : I4497-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

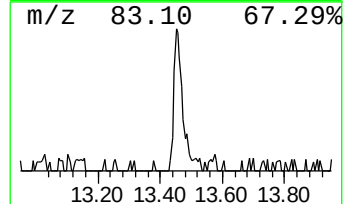
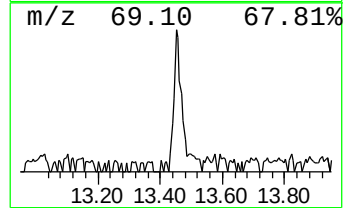
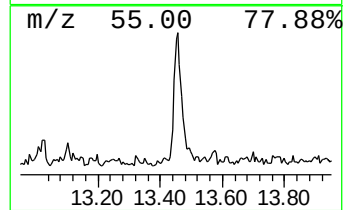
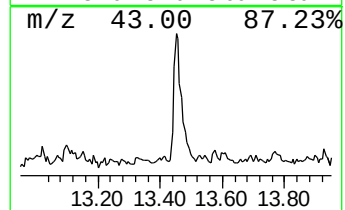
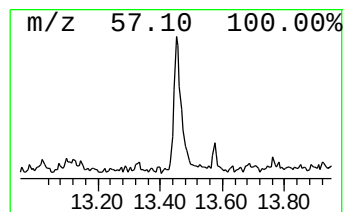
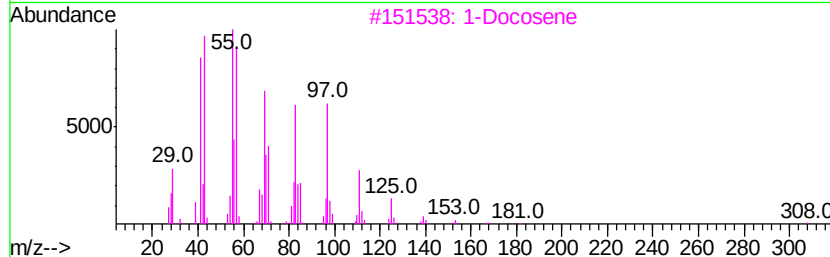
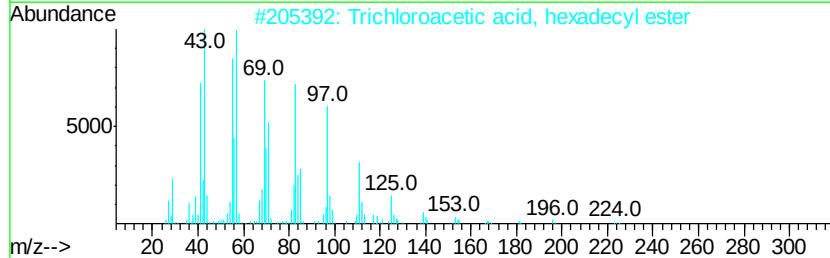
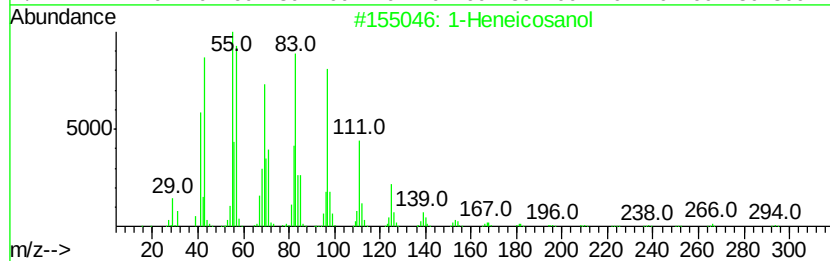
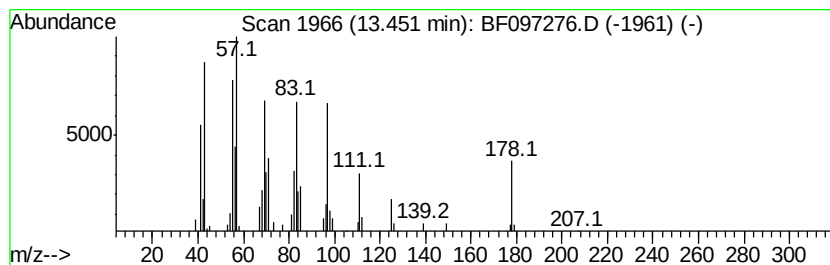
Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.45	3.03 ng	130302	Chrysene-d12	13.57	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
3	1-Docosene	308	C22H44	001599-67-3	93
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080217\
Data File : BF097276.D
Acq On : 2 Aug 2017 16:34
Operator : SJ/JU
Sample : I4497-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

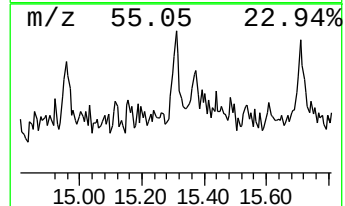
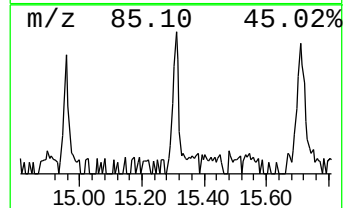
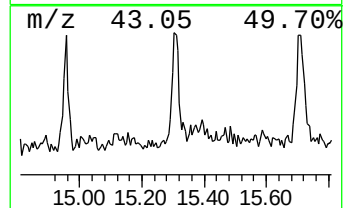
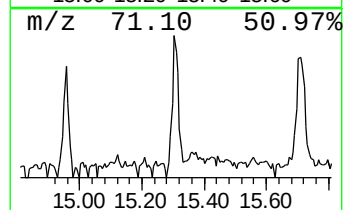
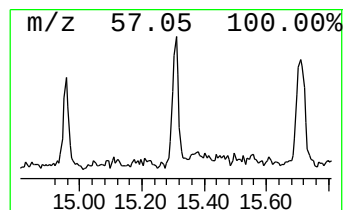
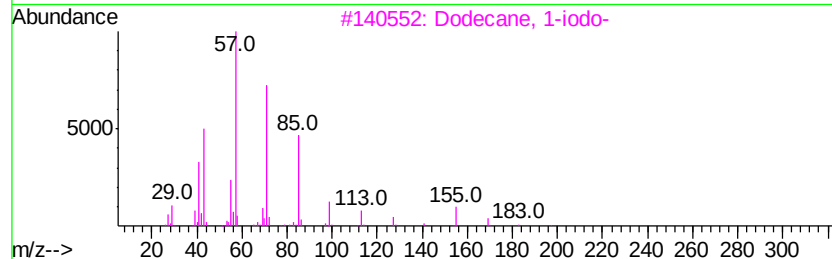
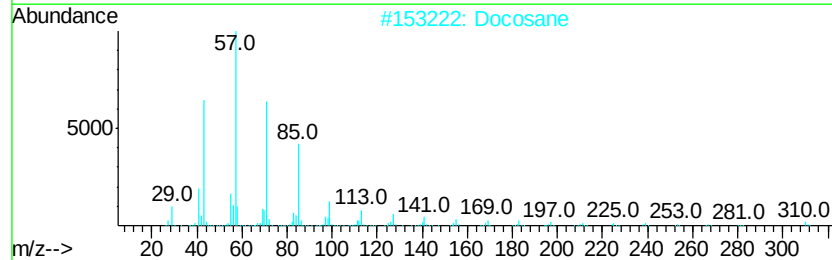
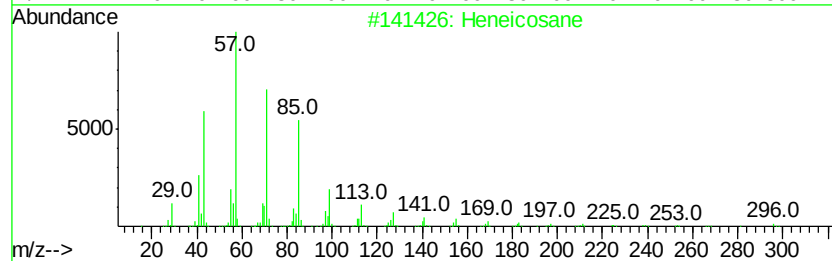
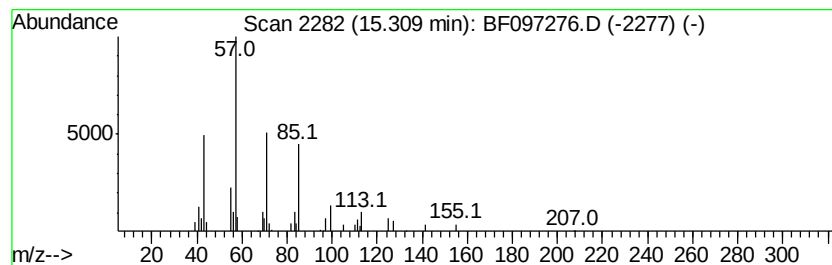
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	2.02 ng	49849	Perylene-d12	14.91

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	87
2	Docosane		310	C22H46	000629-97-0	86
3	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	80
4	Hentriacontane		437	C31H64	000630-04-6	72
5	Pentacosane		352	C25H52	000629-99-2	72



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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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
Propylene Glycol	2.60	11.9	ng	405498	1	6.45	683215	20.0
2-Pentanone, 4-hy...	4.58	13.6	ng	463237	1	6.45	683215	20.0
unknown6.22	6.22	72.0	ng	2459410	1	6.45	683215	20.0
Ethanol, 1-(2-but...	7.66	2.3	ng	110782	2	7.73	952440	20.0
n-Hexadecanoic acid	11.50	3.0	ng	133364	4	10.95	890543	20.0
Octadecanoic acid	12.29	2.1	ng	89206	5	13.57	861383	20.0
1-Heneicosanol	13.45	3.0	ng	130302	5	13.57	861383	20.0
Heneicosane	15.31	2.0	ng	49849	6	14.91	492616	20.0