

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
 Data File : BF099545.D
 Acq On : 16 Oct 2017 15:36
 Operator : SJ/JU
 Sample : I5782-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S1(1-3)

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-BF092317.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	5.069	504	507	521	rBV	314667	384387	19.78%	2.265%
2	5.469	571	575	585	rBV	1812832	1731021	89.08%	10.200%
3	6.481	743	747	760	rBV	1750759	1800651	92.67%	10.610%
4	6.616	766	770	773	rBV	2095199	1770734	91.13%	10.434%
5	6.845	805	809	816	rBV	649982	549776	28.29%	3.239%
6	6.998	831	835	839	rBV	1718031	1434515	73.83%	8.453%
7	7.410	901	905	908	rBV	1219112	1034879	53.26%	6.098%
8	8.128	1023	1027	1030	rBV	793774	706485	36.36%	4.163%
9	8.680	1118	1121	1127	rBB	24845	23082	1.19%	0.136%
10	9.198	1205	1209	1212	rBV	2313642	1943125	100.00%	11.450%
11	9.592	1273	1276	1284	rBV	350372	273745	14.09%	1.613%
12	9.880	1321	1325	1329	rBV	837342	698814	35.96%	4.118%
13	10.592	1443	1446	1452	rBB	70101	55393	2.85%	0.326%
14	10.669	1456	1459	1470	rBV	903077	827161	42.57%	4.874%
15	11.369	1574	1578	1585	rBV	706849	573625	29.52%	3.380%
16	12.951	1843	1847	1850	rBV	1562930	1315968	67.72%	7.754%
17	13.833	1994	1997	2005	rBV	74371	95071	4.89%	0.560%
18	14.015	2024	2028	2033	rBV	516172	510509	26.27%	3.008%
19	14.757	2151	2154	2158	rBV3	17649	24417	1.26%	0.144%
20	14.904	2177	2179	2186	rVB7	17996	24444	1.26%	0.144%
21	15.092	2208	2211	2215	rBV	34844	35840	1.84%	0.211%
22	15.486	2271	2278	2283	rBV	479499	624561	32.14%	3.680%
23	15.904	2343	2349	2355	rBV	61471	106058	5.46%	0.625%
24	16.398	2428	2433	2449	rVB	74123	149674	7.70%	0.882%
25	16.986	2527	2533	2539	rVB	49771	100347	5.16%	0.591%
26	17.674	2644	2650	2659	rVB3	43938	105153	5.41%	0.620%
27	18.497	2785	2790	2800	rVB6	24493	71608	3.69%	0.422%

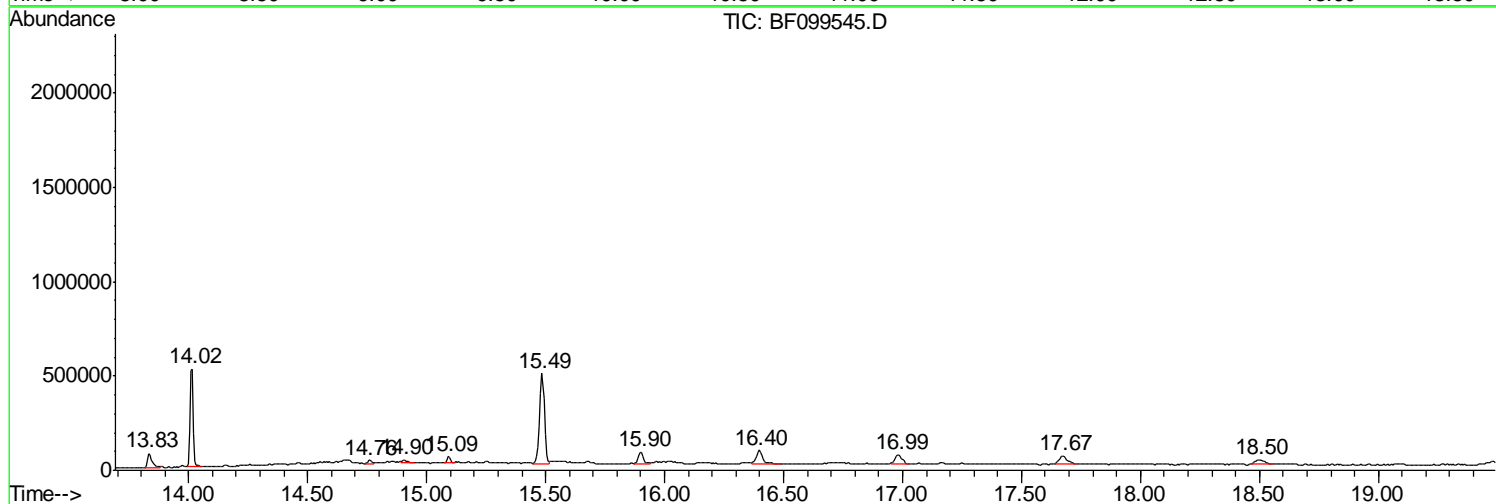
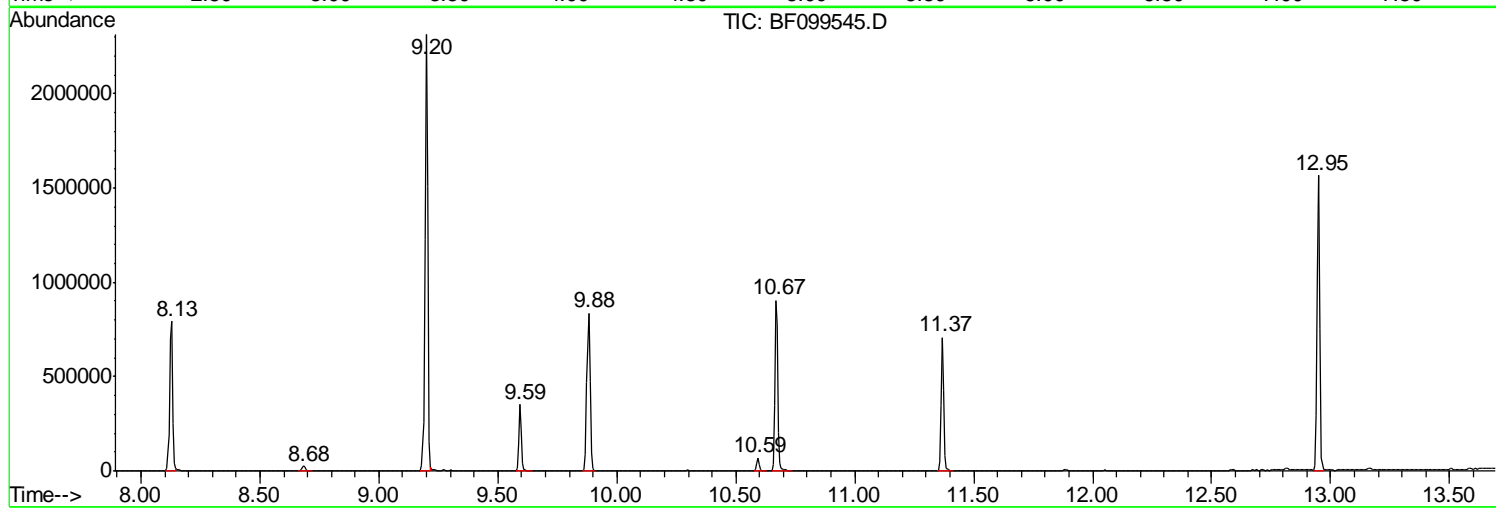
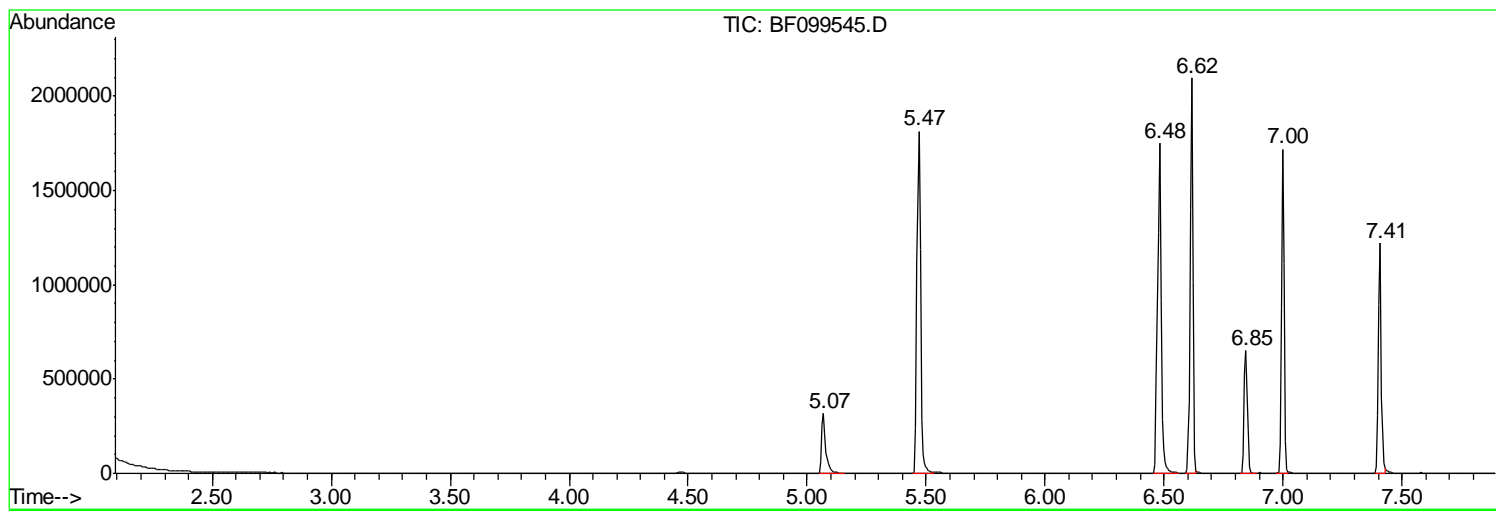
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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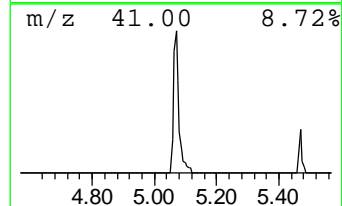
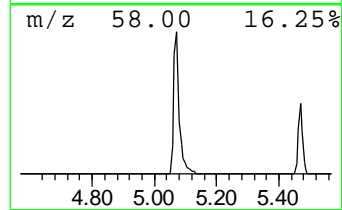
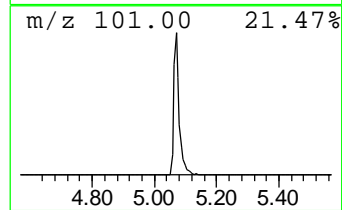
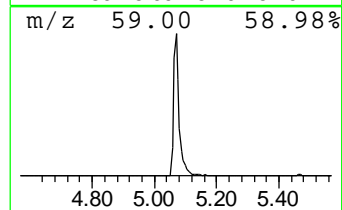
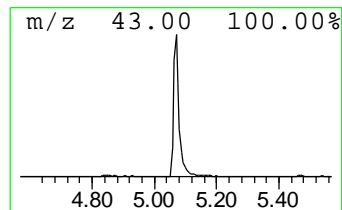
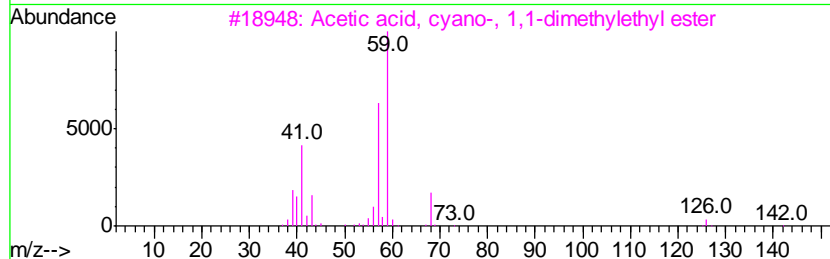
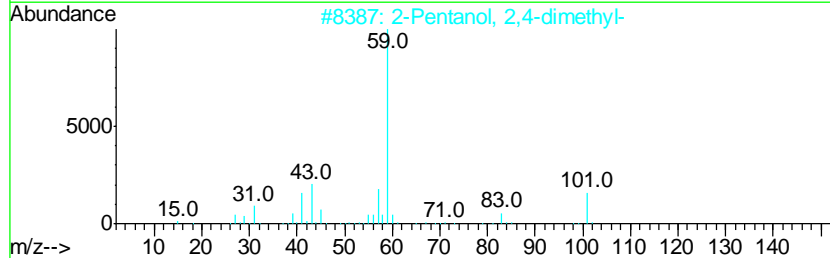
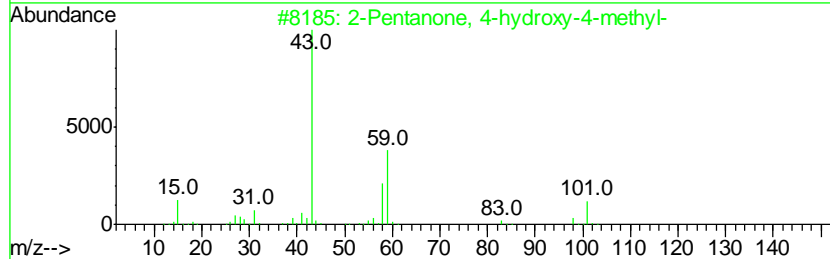
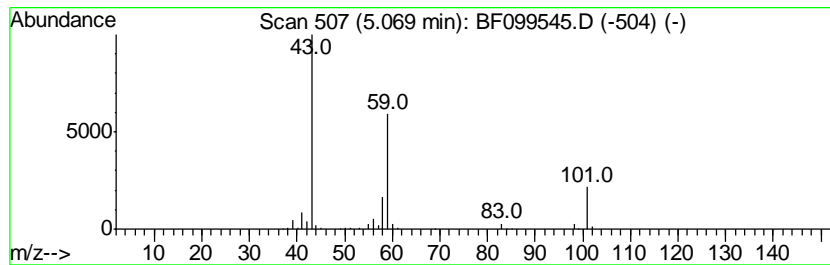
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 Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	13.98 ng	384387	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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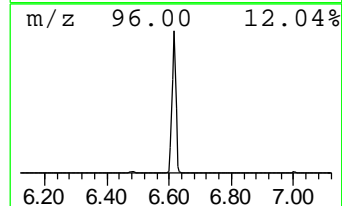
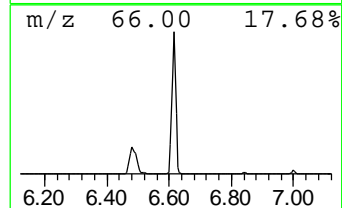
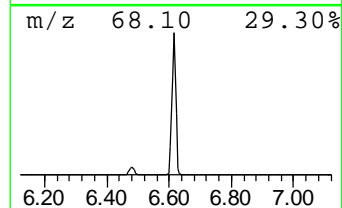
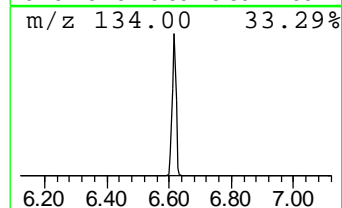
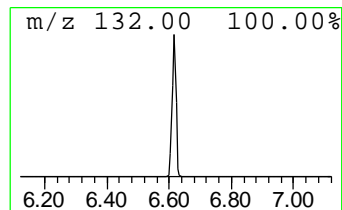
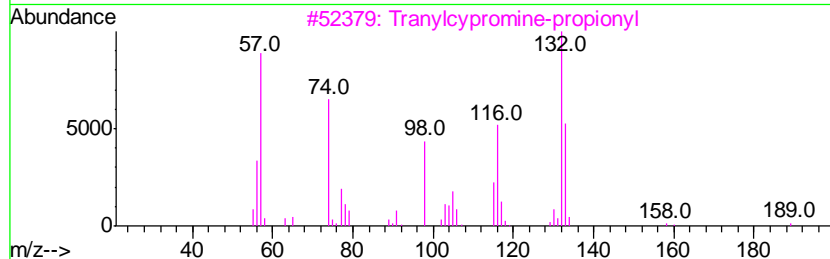
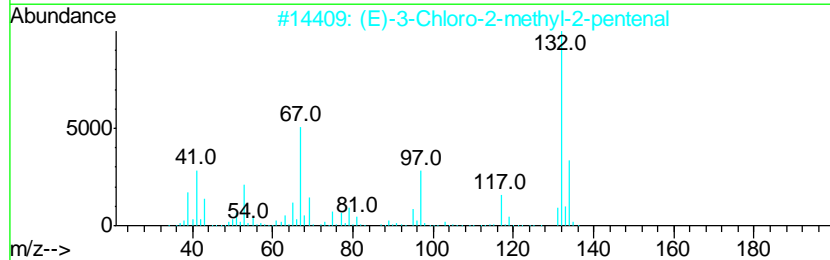
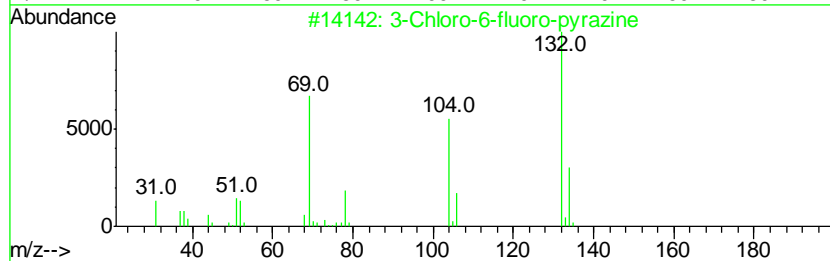
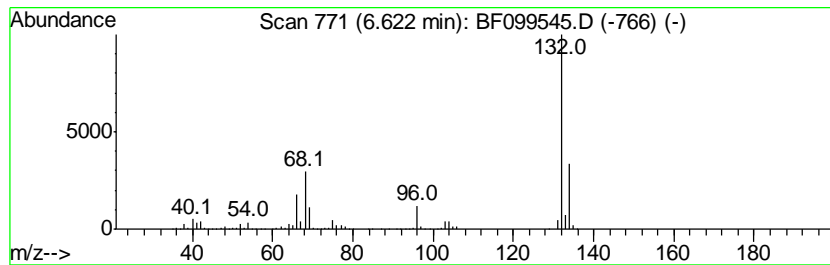
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 Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	64.42 ng	1770730	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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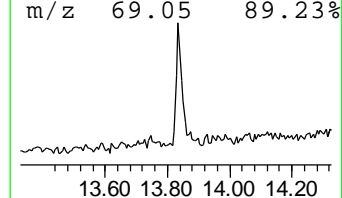
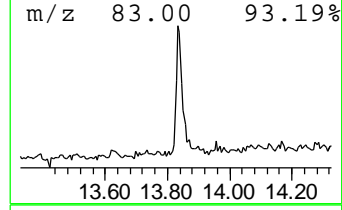
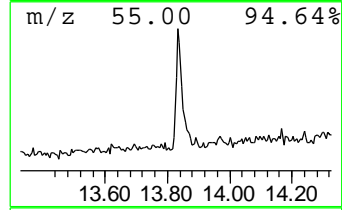
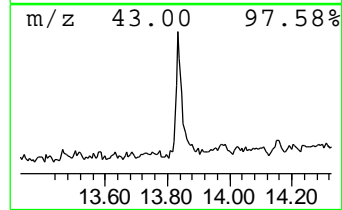
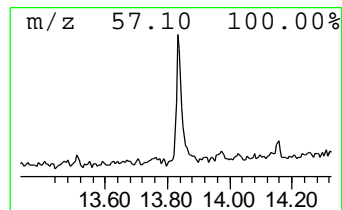
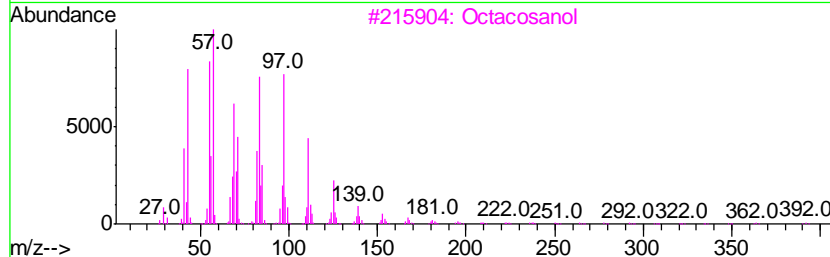
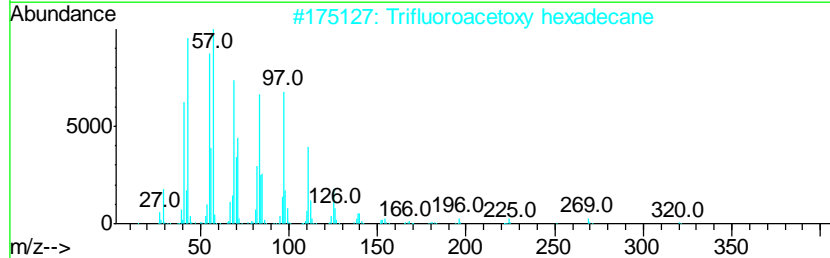
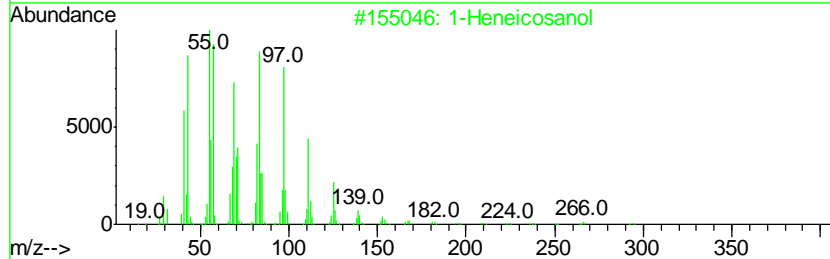
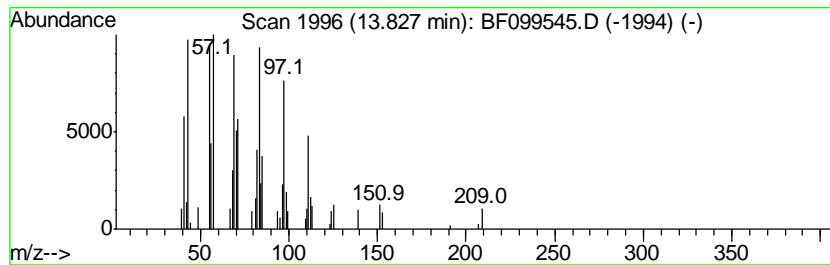
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 Peak Number 4 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	3.72 ng	95071	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	94
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3		Octacosanol	410	C28H58O	000557-61-9	93
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
5		Behenic alcohol	326	C22H46O	000661-19-8	93



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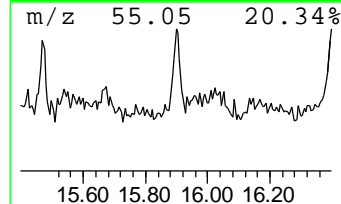
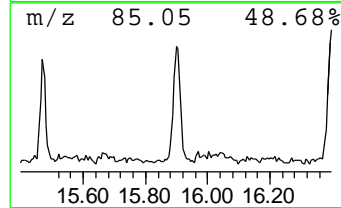
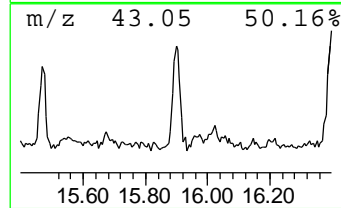
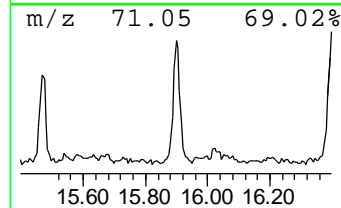
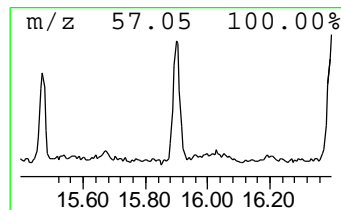
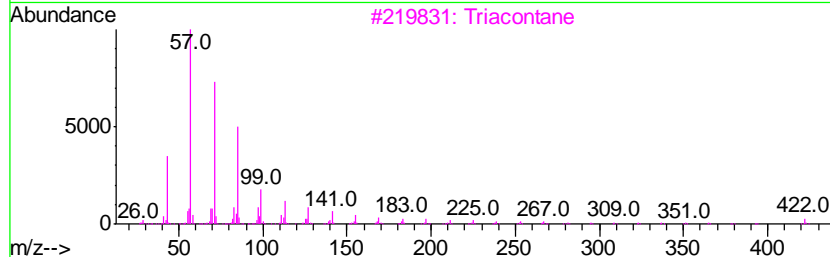
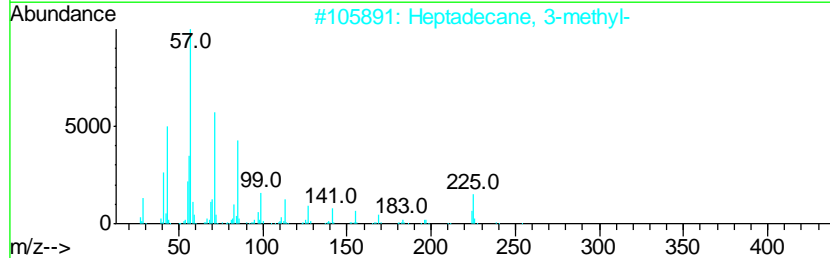
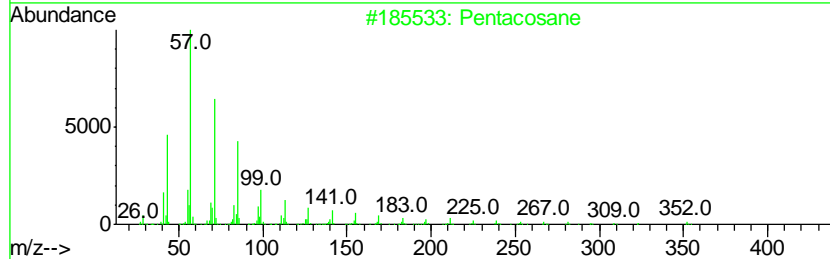
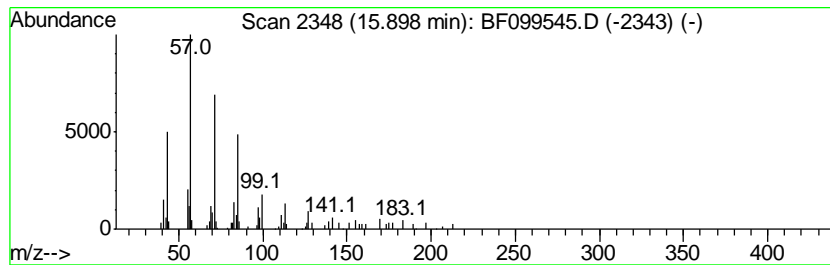
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TIC Library : C:\DATABASE\NIST11.L
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 Peak Number 5 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	3.40 ng	106058	Perylene-d12	15.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentacosane	352	C25H52	000629-99-2	91
2		Heptadecane, 3-methyl-	254	C18H38	006418-44-6	91
3		Triacontane	422	C30H62	000638-68-6	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Heptacosane	380	C27H56	000593-49-7	90



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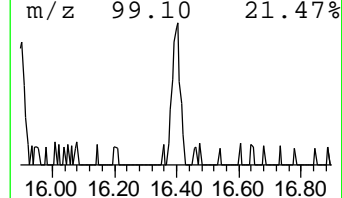
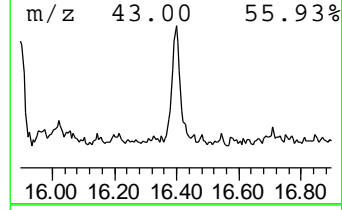
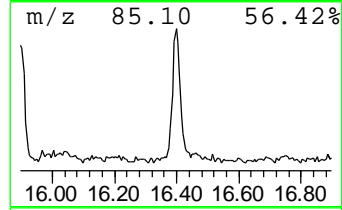
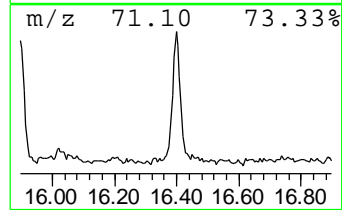
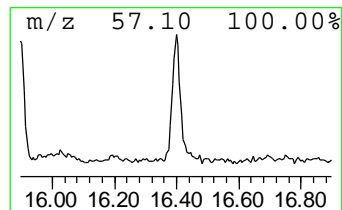
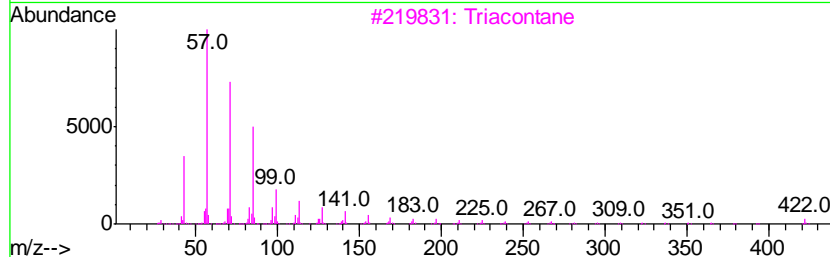
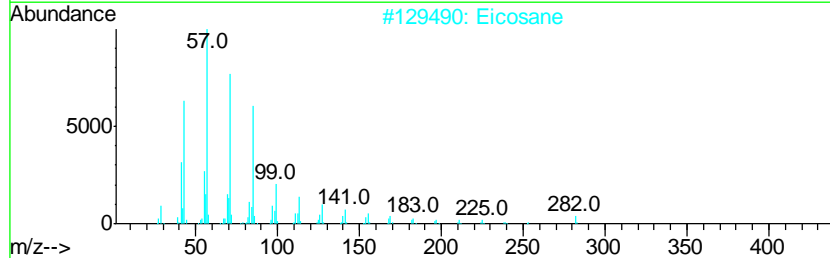
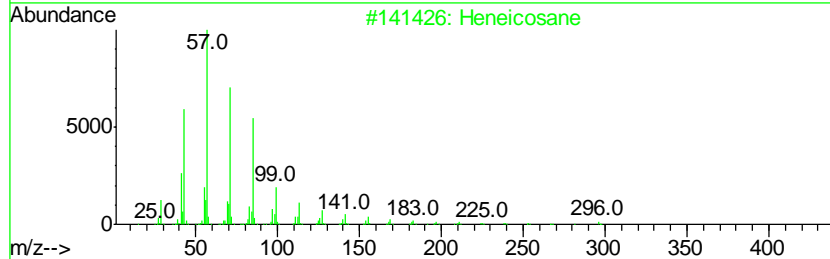
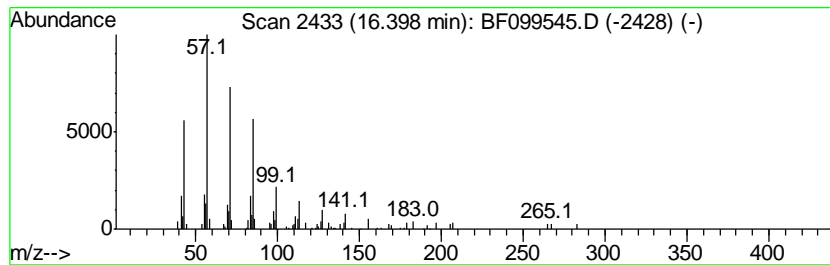
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 Peak Number 6 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	4.79 ng	149674	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Eicosane	282	C20H42	000112-95-8	91
3		Triacotane	422	C30H62	000638-68-6	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5		Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	90



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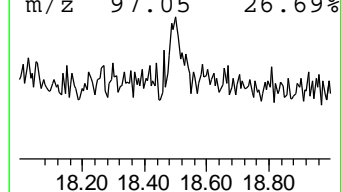
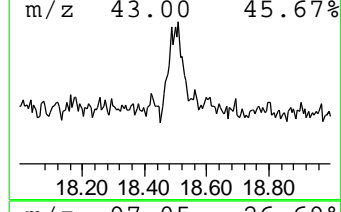
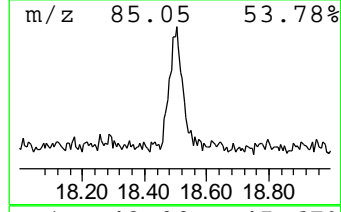
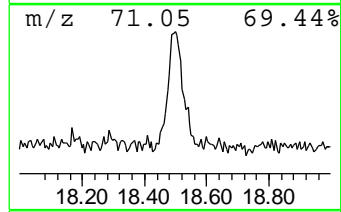
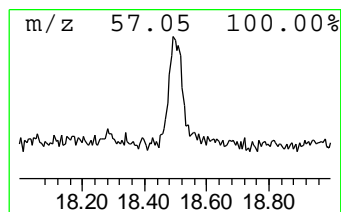
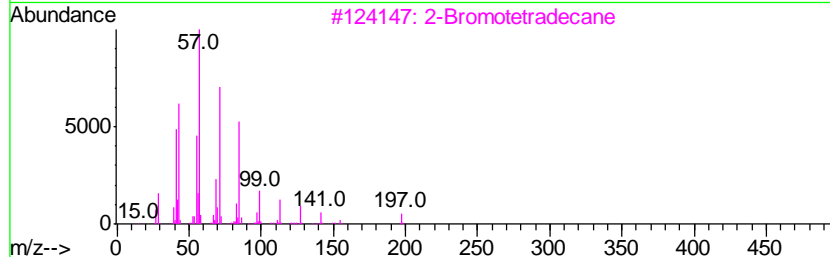
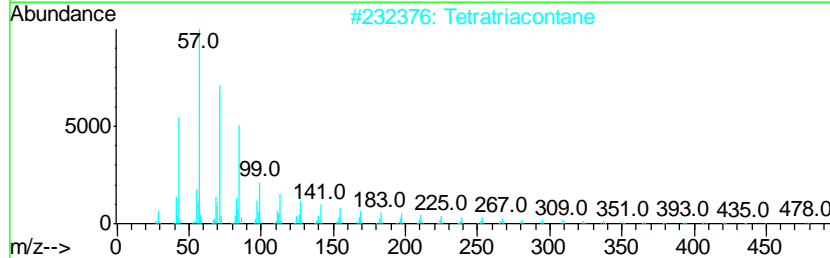
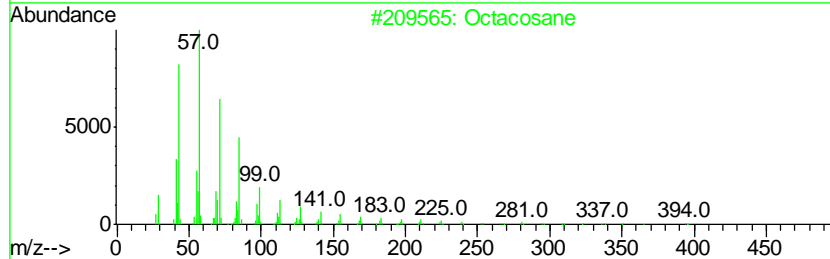
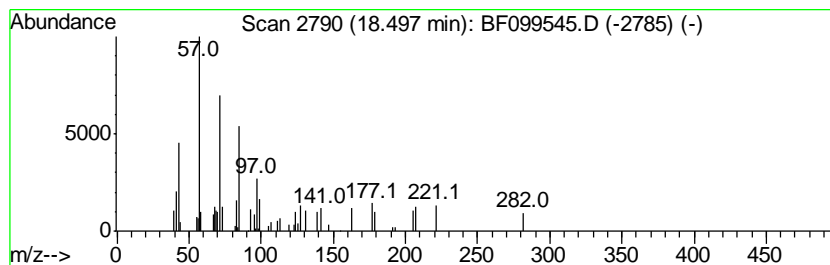
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 unknown18.50 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.50	2.29 ng	71608	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	38
2		Tetratriacontane	479	C34H70	014167-59-0	38
3		2-Bromotetradecane	276	C14H29Br	074036-95-6	38
4		Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	38
5		Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101617\
Data File : BF099545.D
Acq On : 16 Oct 2017 15:36
Operator : SJ/JU
Sample : I5782-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S1(1-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	5.07	14.0	ng	384387	1	6.85	549776	20.0
unknown6.62	6.62	64.4	ng	1770730	1	6.85	549776	20.0
1-Heneicosanol	13.83	3.7	ng	95071	5	14.02	510509	20.0
Pentacosane	15.90	3.4	ng	106058	6	15.49	624561	20.0
Heneicosane	16.40	4.8	ng	149674	6	15.49	624561	20.0
unknown18.50	18.50	2.3	ng	71608	6	15.49	624561	20.0