

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072817\
 Data File : BF097171.D
 Acq On : 28 Jul 2017 23:18
 Operator : SJ/JU
 Sample : I4456-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-10D56

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	4.634	462	467	482	rBV	584841	889669	27.43%	3.614%
2	5.093	540	545	569	rBV	2433946	2939693	90.62%	11.941%
3	6.157	721	726	740	rBV	2831873	3243905	100.00%	13.177%
4	6.263	740	744	755	rVB	2902230	2800320	86.33%	11.375%
5	6.487	779	782	787	rBV	945570	777708	23.97%	3.159%
6	6.645	804	809	812	rBV	2098653	2040128	62.89%	8.287%
7	7.057	874	879	882	rBV	1933784	1784294	55.00%	7.248%
8	7.769	996	1000	1008	rBV	1133358	999950	30.83%	4.062%
9	8.845	1179	1183	1187	rBV	2314600	2216249	68.32%	9.003%
10	9.245	1247	1251	1256	rBV	595704	467331	14.41%	1.898%
11	9.516	1292	1297	1300	rBV	979736	924627	28.50%	3.756%
12	9.751	1334	1337	1341	rBV	41763	40778	1.26%	0.166%
13	10.298	1426	1430	1436	rBV	1044702	953157	29.38%	3.872%
14	10.439	1451	1454	1462	rBV	42526	49214	1.52%	0.200%
15	10.886	1521	1530	1532	rBV2	32676	39752	1.23%	0.161%
16	10.986	1543	1547	1550	rBV	796463	696462	21.47%	2.829%
17	11.010	1550	1551	1555	rVB	86284	53556	1.65%	0.218%
18	12.192	1749	1752	1756	rBV	81637	69268	2.14%	0.281%
19	12.416	1785	1790	1796	rBV	72893	74982	2.31%	0.305%
20	12.569	1812	1816	1820	rBV	1353222	1267290	39.07%	5.148%
21	13.480	1968	1971	1977	rBV2	53088	69189	2.13%	0.281%
22	13.610	1986	1993	1996	rBV	747463	725875	22.38%	2.949%
23	14.104	2074	2077	2081	rBV3	50596	61254	1.89%	0.249%
24	14.604	2159	2162	2169	rVB	42606	62658	1.93%	0.255%
25	14.692	2174	2177	2180	rBV2	42610	45183	1.39%	0.184%
26	14.762	2186	2189	2192	rBV3	40269	53561	1.65%	0.218%
27	14.962	2218	2223	2227	rVV	469117	551120	16.99%	2.239%
28	15.010	2227	2231	2236	rVB2	70622	96901	2.99%	0.394%
29	15.362	2287	2291	2295	rBV	90807	125811	3.88%	0.511%
30	15.774	2355	2361	2369	rBV	102842	183640	5.66%	0.746%
31	16.251	2436	2442	2447	rBV2	61617	116722	3.60%	0.474%
32	16.815	2532	2538	2544	rVB2	57969	131542	4.06%	0.534%
33	18.256	2777	2783	2786	rBV7	31106	66033	2.04%	0.268%

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ALS Vial : 15 Sample Multiplier: 1

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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-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

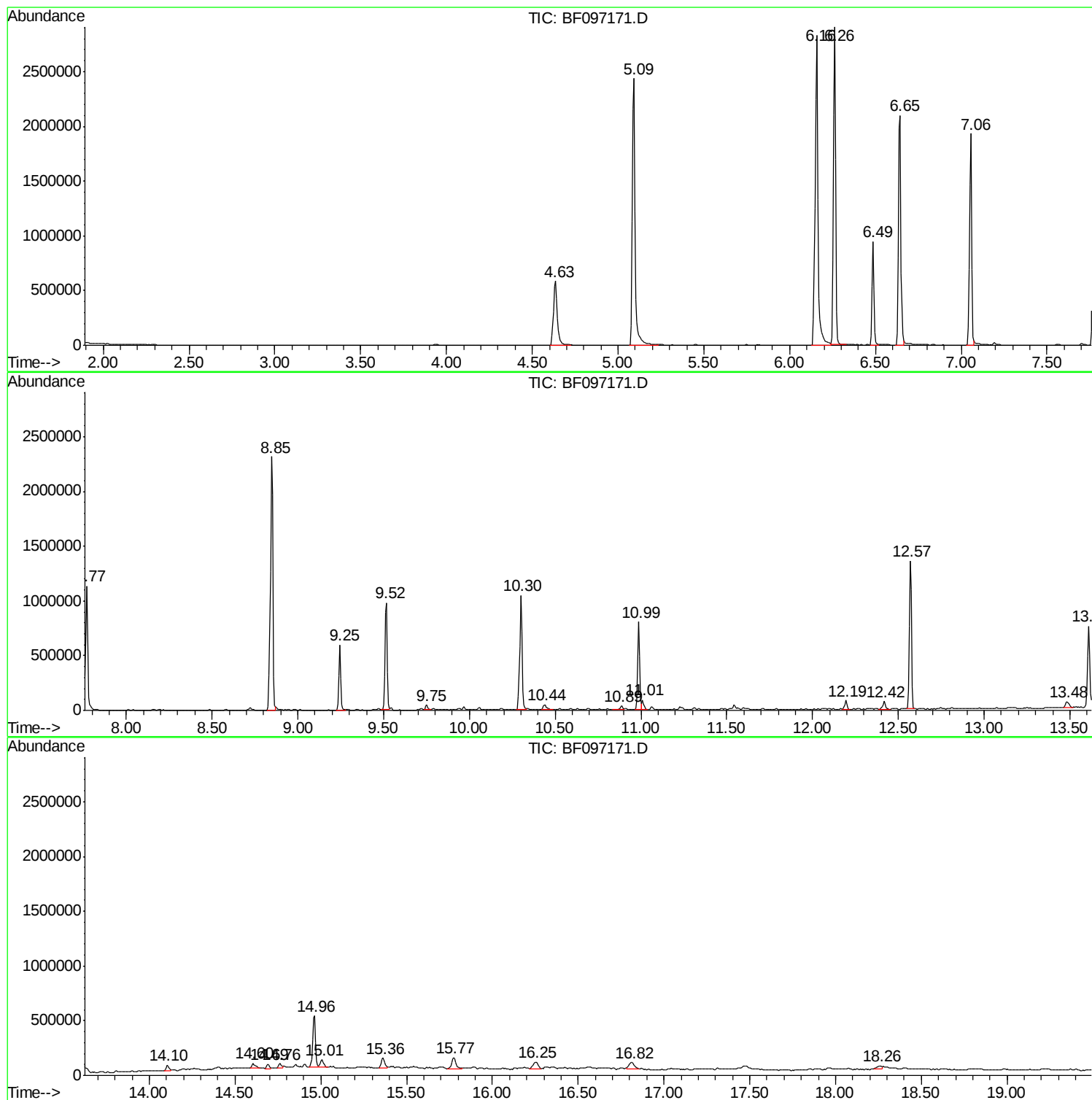
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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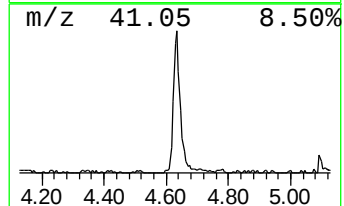
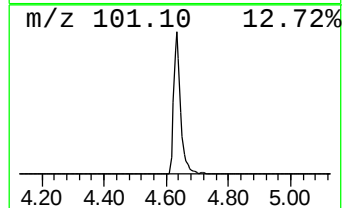
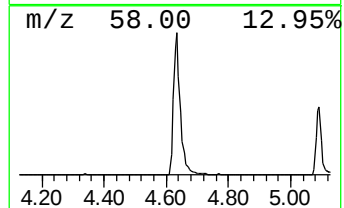
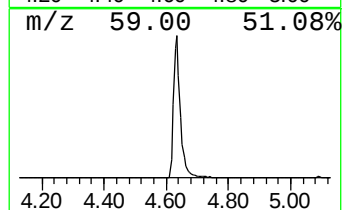
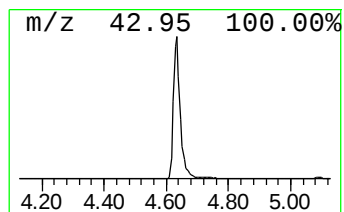
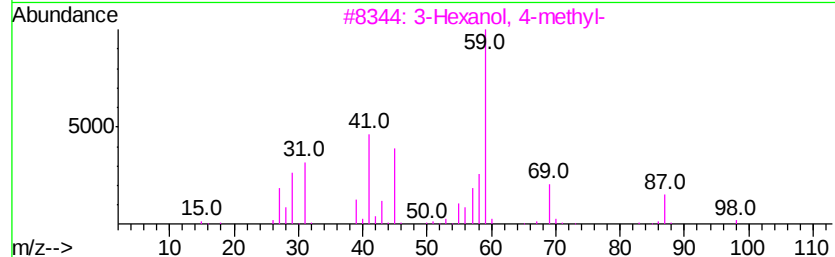
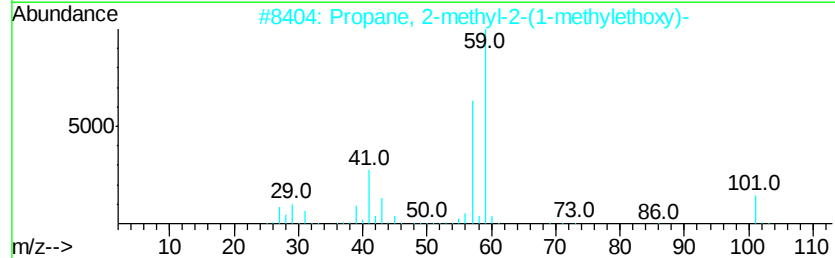
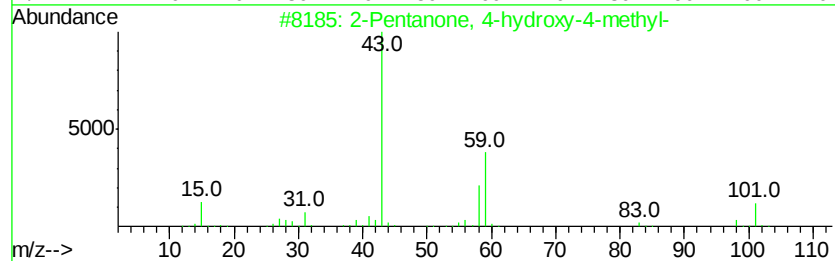
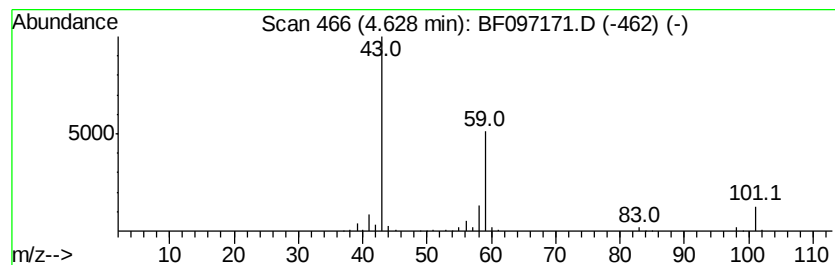
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	22.88 ng	889669	1,4-Dichlorobenzene-d4	6.49

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		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5		3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9



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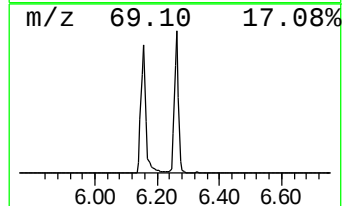
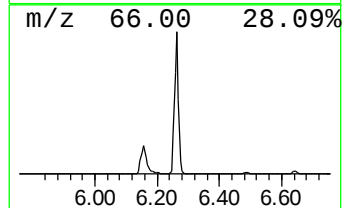
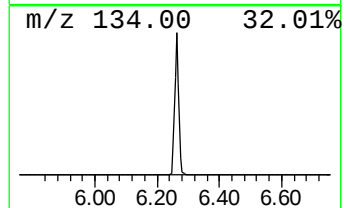
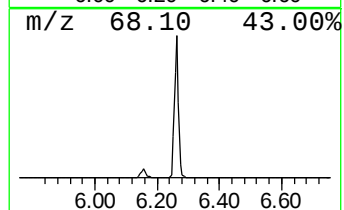
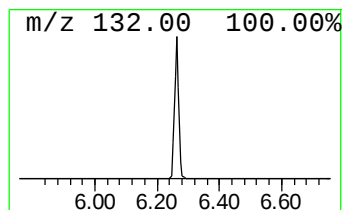
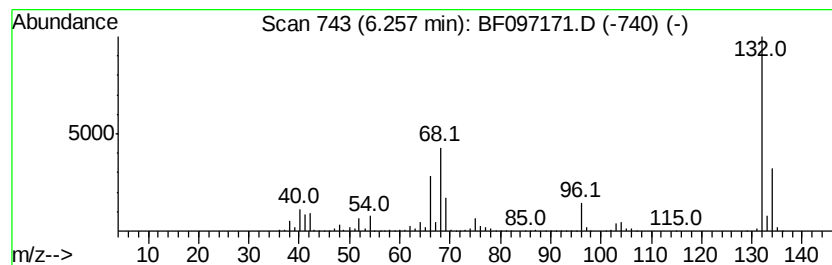
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	72.01 ng	2800320	1,4-Dichlorobenzene-d4	6.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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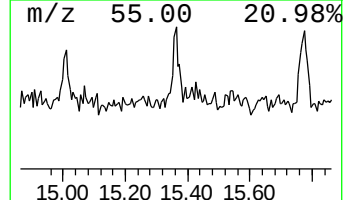
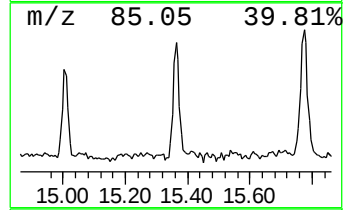
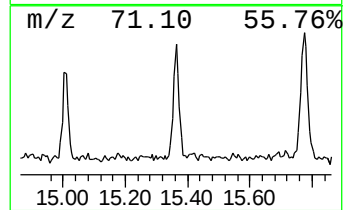
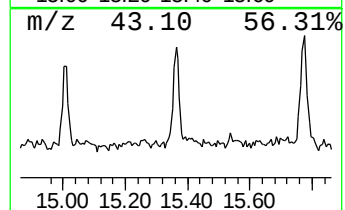
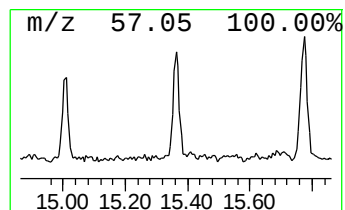
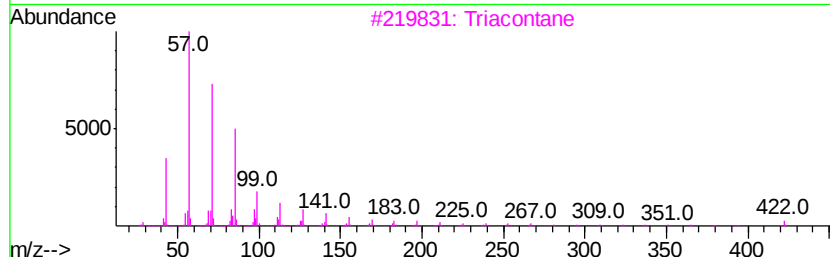
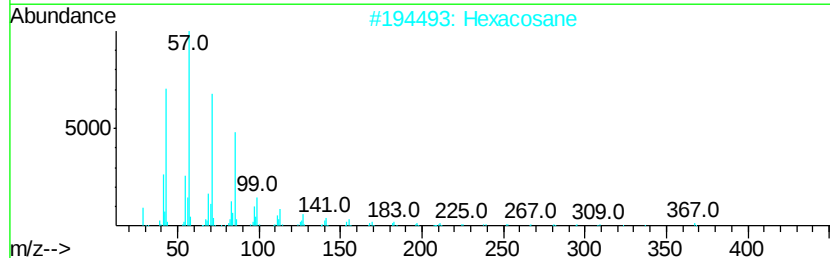
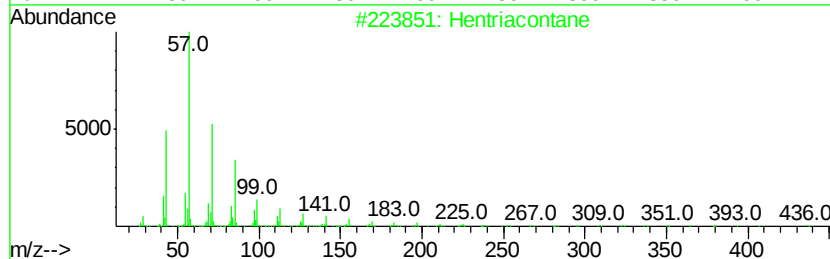
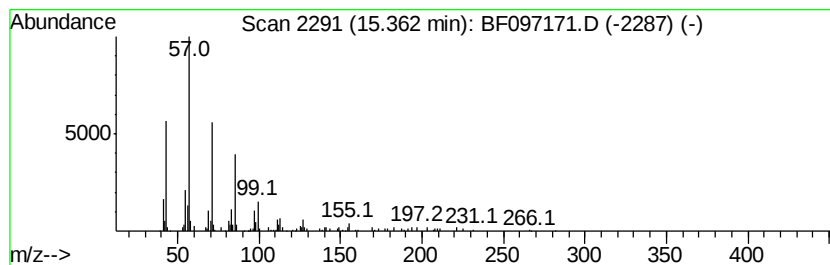
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	4.57 ng	125811	Perylene-d12	14.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	90
2	Hexacosane		366	C26H54	000630-01-3	86
3	triacontane		422	C30H62	000638-68-6	80
4	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	80
5	Hexadecane		226	C16H34	000544-76-3	80



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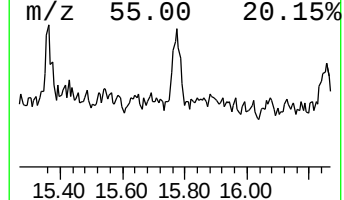
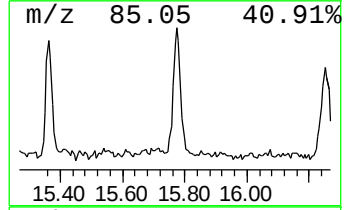
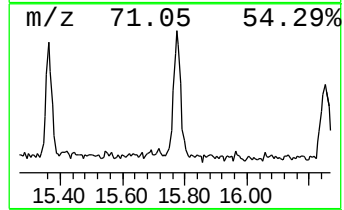
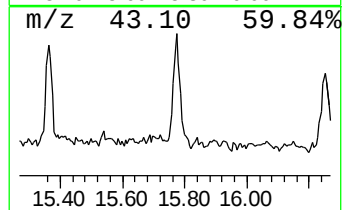
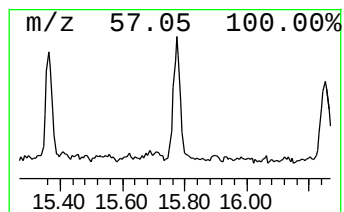
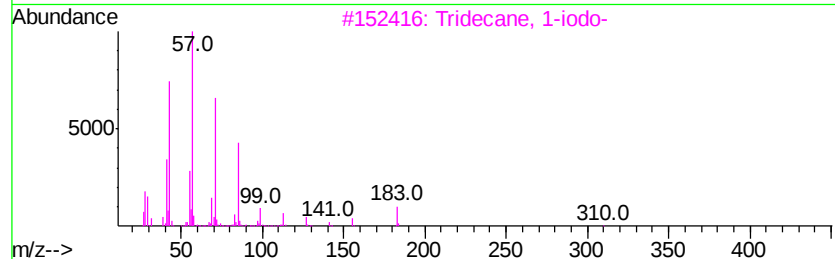
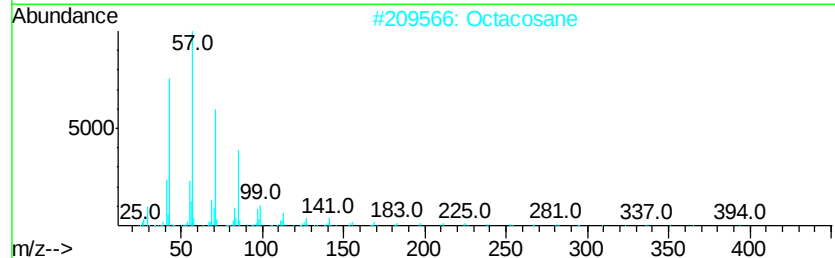
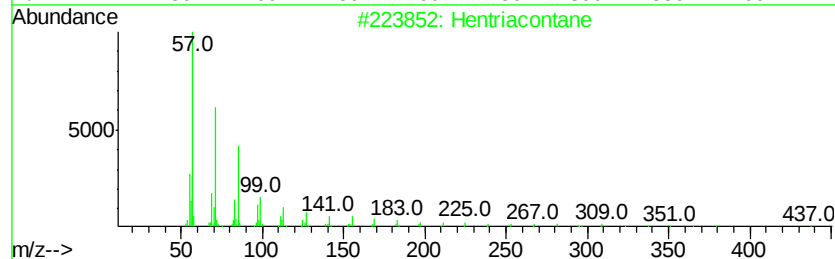
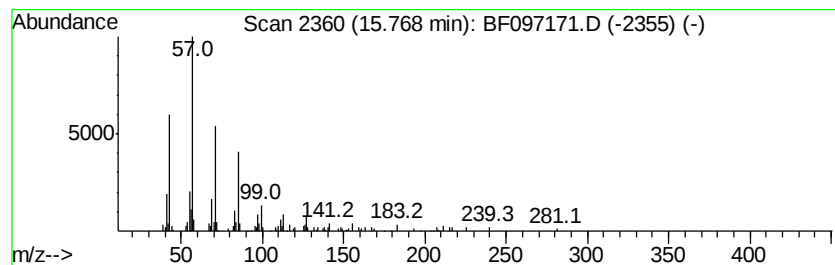
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Tridecane, 1-iodo- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	6.66 ng	183640	Perylene-d12	14.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hentriacontane	437	C31H64	000630-04-6	91
2		Octacosane	394	C28H58	000630-02-4	90
3		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
4		Eicosane	282	C20H42	000112-95-8	86
5		Heptacosane	380	C27H56	000593-49-7	86



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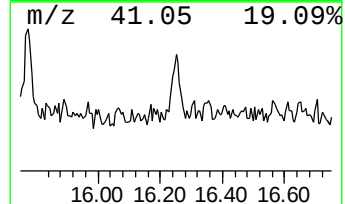
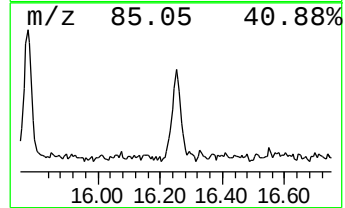
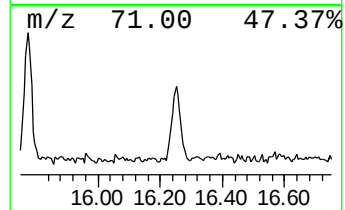
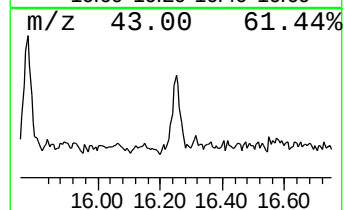
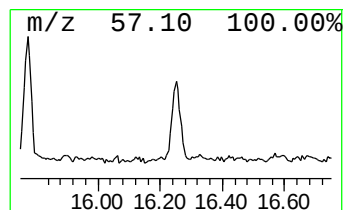
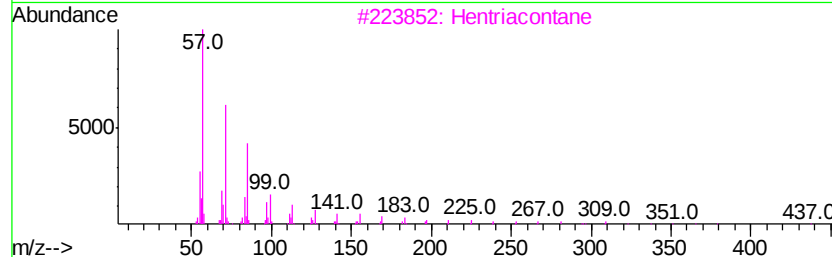
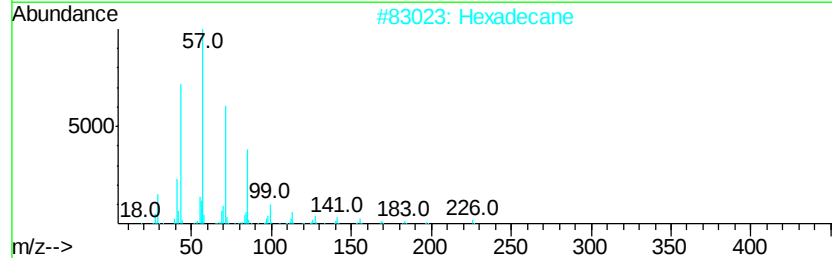
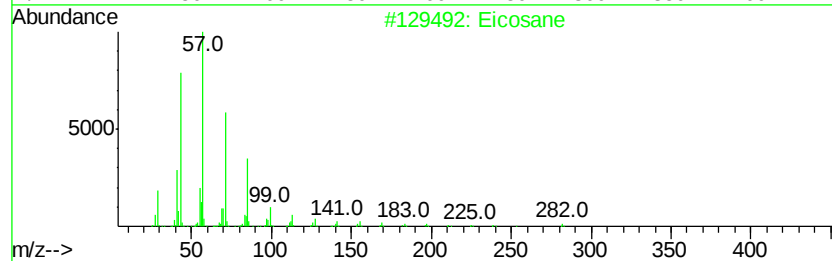
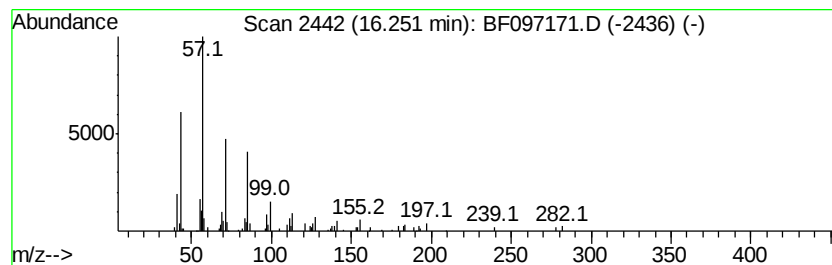
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.25	4.24 ng	116722	Perylene-d12	14.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	90
2	Hexadecane		226	C16H34	000544-76-3	78
3	Hentriacontane		437	C31H64	000630-04-6	78
4	Pentacosane		352	C25H52	000629-99-2	74
5	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	72



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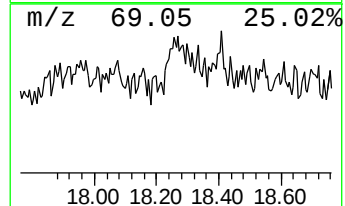
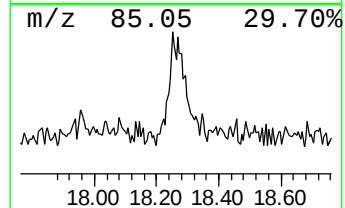
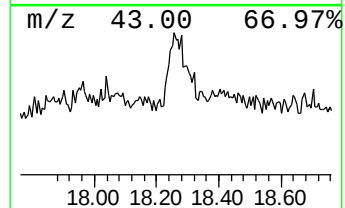
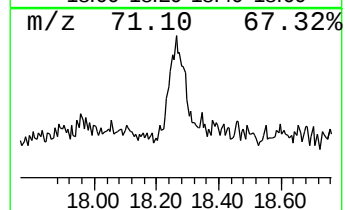
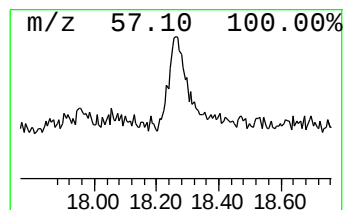
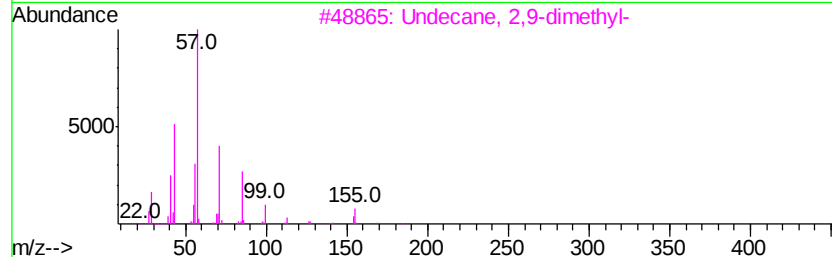
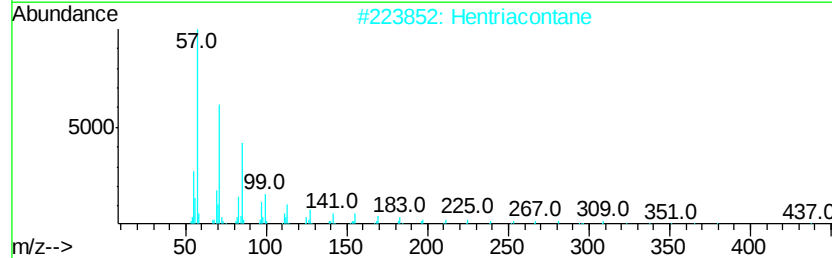
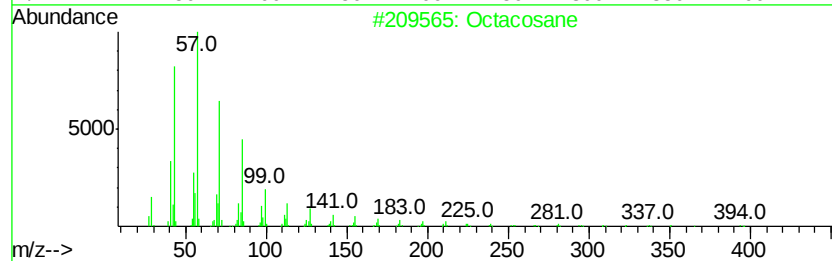
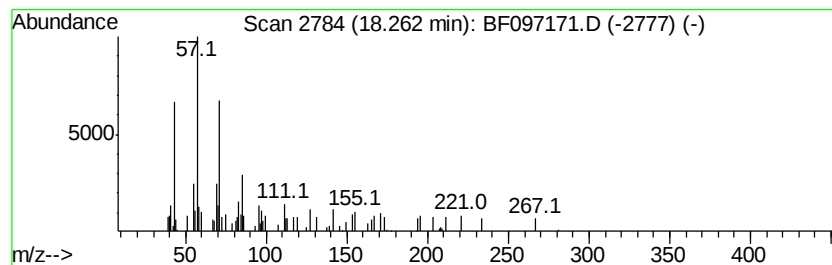
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown18.26 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	2.40 ng	66033	Perylene-d12	14.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	47
2		Hentriacontane	437	C31H64	000630-04-6	47
3		Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	47
4		Tetracosane	338	C24H50	000646-31-1	47
5		Tetradecane	198	C14H30	000629-59-4	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072817\
Data File : BF097171.D
Acq On : 28 Jul 2017 23:18
Operator : SJ/JU
Sample : I4456-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-10D56

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
2-Pentanone, 4-hy...	4.63	22.9	ng	889669	1	6.49	777708	20.0
unknown6.26	6.26	72.0	ng	2800320	1	6.49	777708	20.0
Hentriacontane	15.36	4.6	ng	125811	6	14.96	551120	20.0
Tridecane, 1-iodo-	15.77	6.7	ng	183640	6	14.96	551120	20.0
Eicosane	16.25	4.2	ng	116722	6	14.96	551120	20.0
unknown18.26	18.26	2.4	ng	66033	6	14.96	551120	20.0