

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071717\
 Data File : BF096826.D
 Acq On : 17 Jul 2017 18:23
 Operator : SJ/JU
 Sample : I4203-03
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NB-SB02A

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-BF071317.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	4.781	471	475	484	rBV	167175	235581	10.60%	1.207%
2	5.216	545	549	561	rVB	2063943	2148447	96.68%	11.008%
3	6.263	722	727	739	rBV	2133108	2222321	100.00%	11.387%
4	6.381	743	747	751	rBV	2180669	2133193	95.99%	10.930%
5	6.610	782	786	790	rBV	699120	554119	24.93%	2.839%
6	6.769	808	813	816	rBV	1845301	1613578	72.61%	8.268%
7	7.175	877	882	885	rBV	1465641	1337352	60.18%	6.852%
8	7.892	1000	1004	1007	rBV	913828	742767	33.42%	3.806%
9	8.969	1182	1187	1190	rBV	2403372	2094766	94.26%	10.733%
10	9.357	1250	1253	1256	rBV	238356	202767	9.12%	1.039%
11	9.639	1296	1301	1304	rBV	701296	670992	30.19%	3.438%
12	10.086	1374	1377	1381	rBV	47689	35430	1.59%	0.182%
13	10.422	1430	1434	1437	rBV	1028792	923956	41.58%	4.734%
14	10.557	1454	1457	1467	rBV	52702	67425	3.03%	0.345%
15	11.110	1547	1551	1554	rBV	613530	499303	22.47%	2.558%
16	11.657	1641	1644	1651	rVB	47119	47522	2.14%	0.243%
17	12.316	1752	1756	1759	rBV	39424	35929	1.62%	0.184%
18	12.527	1788	1792	1796	rBV2	34973	54809	2.47%	0.281%
19	12.574	1796	1800	1811	rVB	238389	308980	13.90%	1.583%
20	12.692	1816	1820	1824	rVB	1610623	1513347	68.10%	7.754%
21	13.280	1918	1920	1926	rVB	32876	35103	1.58%	0.180%
22	13.598	1969	1974	1985	rBV2	172723	239316	10.77%	1.226%
23	13.733	1993	1997	2005	rVB	667601	625598	28.15%	3.205%
24	13.845	2012	2016	2021	rBV7	20862	38833	1.75%	0.199%
25	13.927	2026	2030	2032	rBV	39519	37685	1.70%	0.193%
26	14.227	2078	2081	2090	rBV2	46786	55108	2.48%	0.282%
27	14.498	2123	2127	2128	rBV4	17708	25731	1.16%	0.132%
28	14.521	2128	2131	2134	rVV2	39215	43065	1.94%	0.221%
29	14.586	2140	2142	2145	rVB3	32780	25135	1.13%	0.129%
30	14.727	2163	2166	2171	rBV	36783	55273	2.49%	0.283%
31	14.821	2179	2182	2185	rVB2	53715	52067	2.34%	0.267%
32	14.992	2209	2211	2217	rBV2	32078	44533	2.00%	0.228%
33	15.104	2226	2230	2235	rVB	480517	571734	25.73%	2.929%
34	15.157	2236	2239	2243	rVB2	42583	42851	1.93%	0.220%

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Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	15.539	2301	2304	2308	rVB	32524	41991	1.89%	0.215%
36	15.733	2333	2337	2340	rBV6	17784	34548	1.55%	0.177%
37	15.986	2376	2380	2383	rVB2	28771	38584	1.74%	0.198%
38	17.098	2564	2569	2575	rBV6	19027	42803	1.93%	0.219%
39	17.809	2686	2690	2692	rBV5	17180	23954	1.08%	0.123%

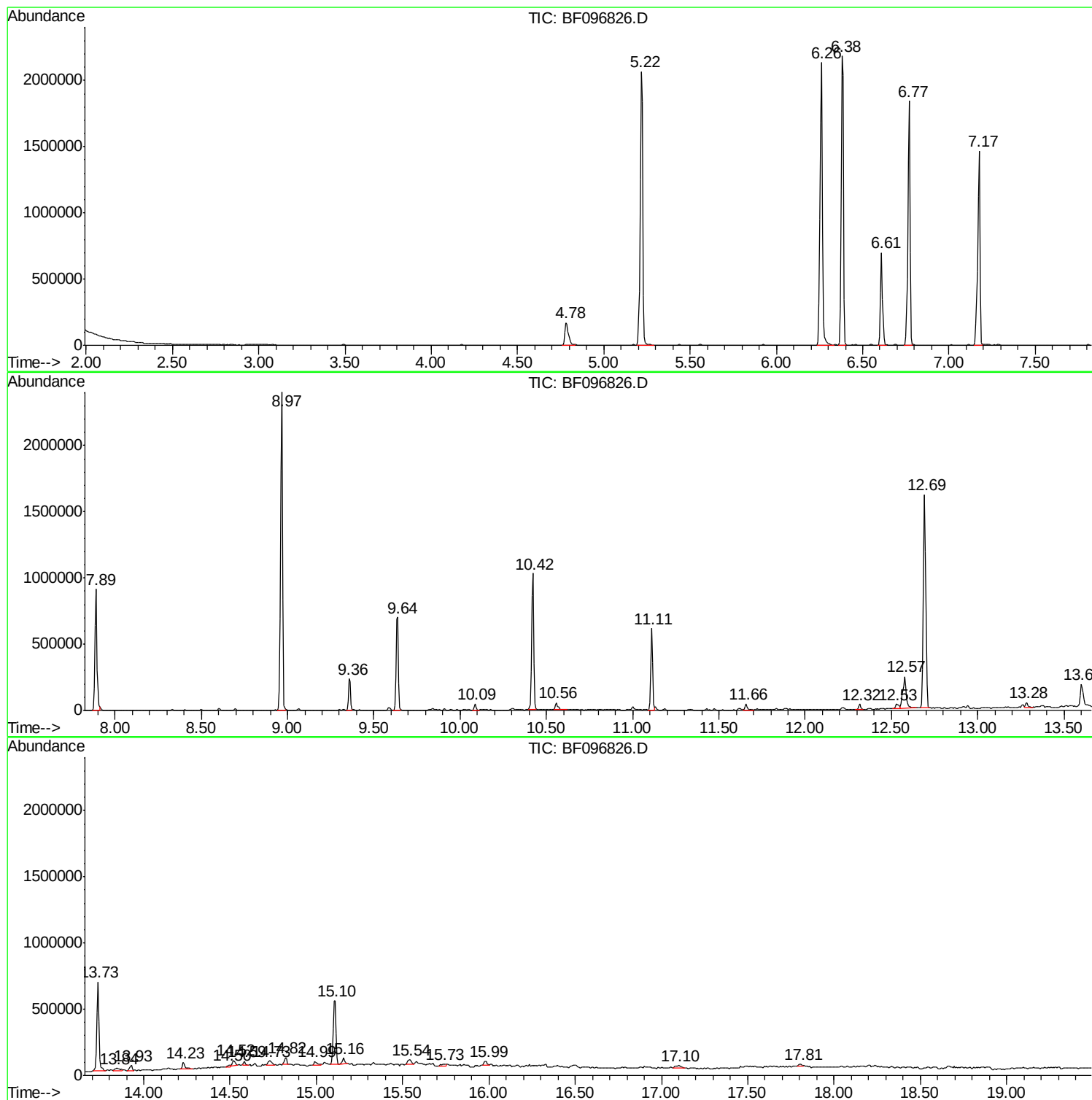
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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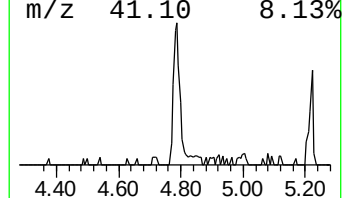
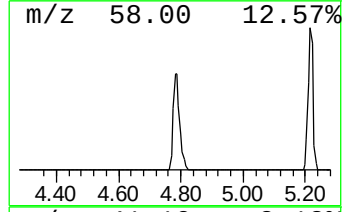
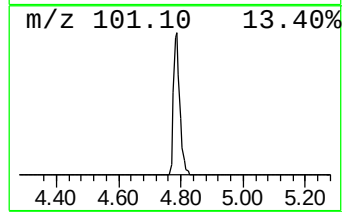
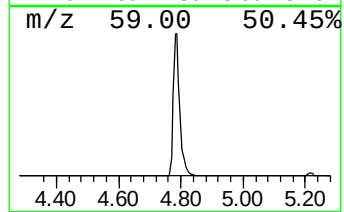
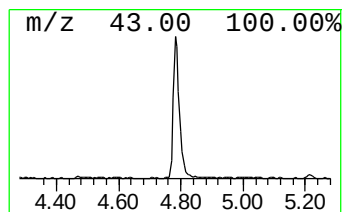
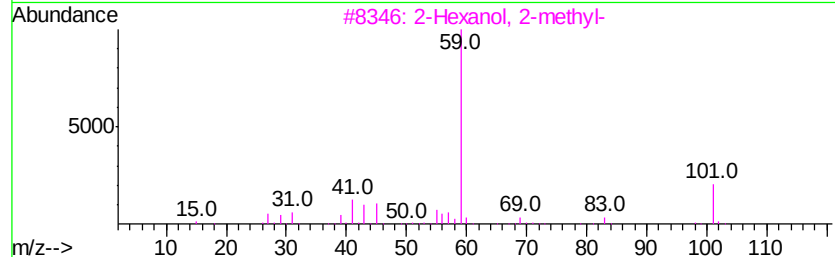
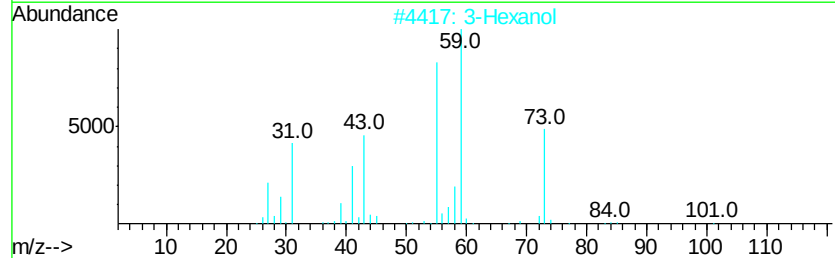
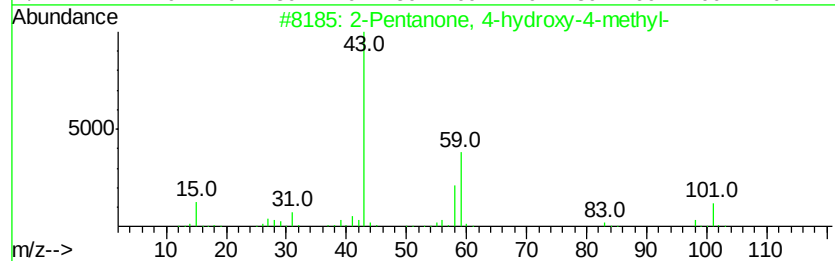
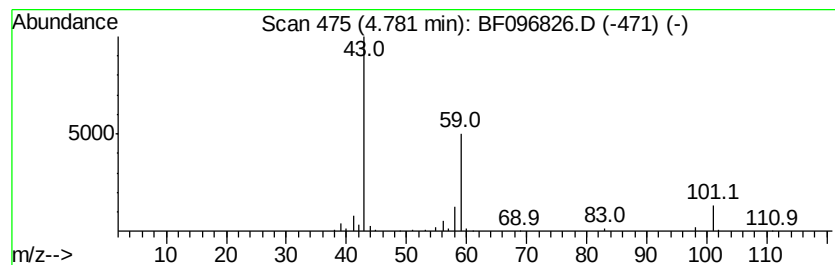
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	8.50 ng	235581	1,4-Dichlorobenzene-d4	6.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol	102	C6H14O	000623-37-0	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
5	3-Pentanol	88	C5H12O	000584-02-1	9



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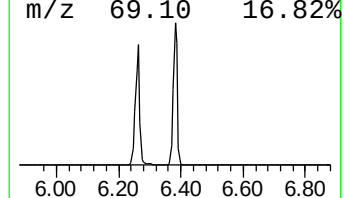
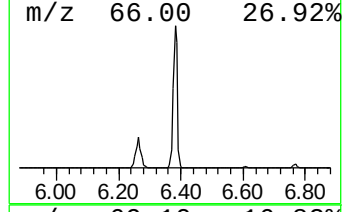
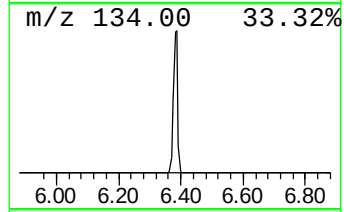
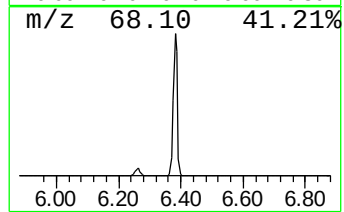
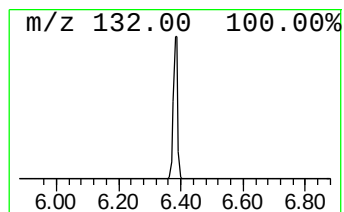
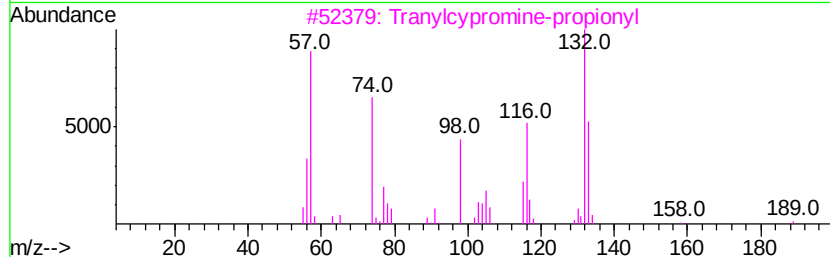
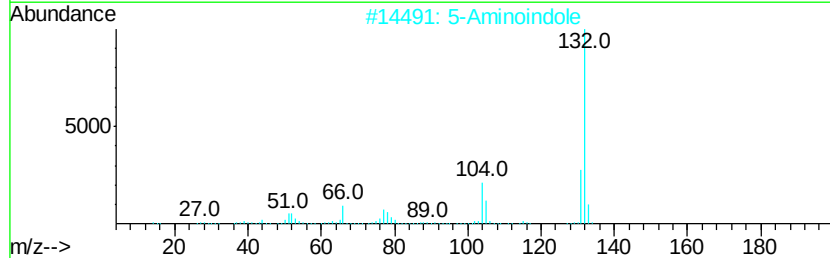
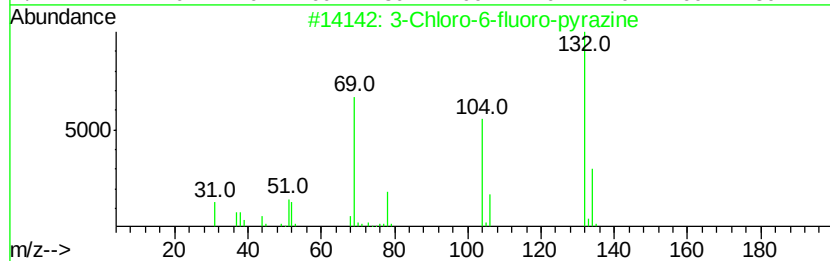
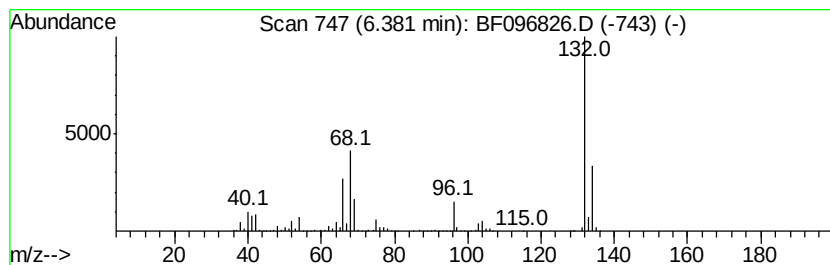
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.38	76.99 ng	2133190	1,4-Dichlorobenzene-d4	6.61

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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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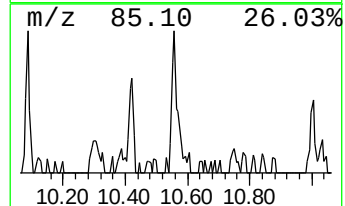
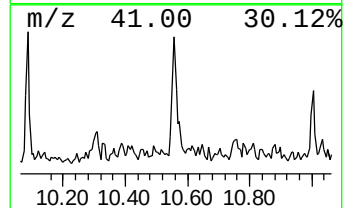
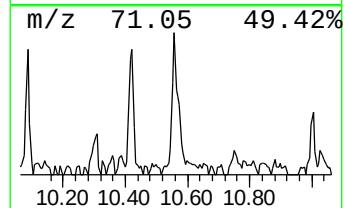
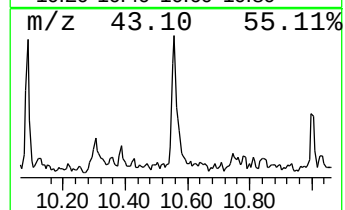
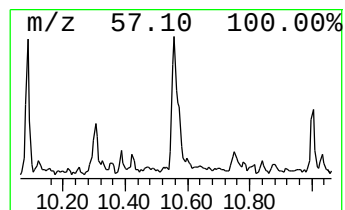
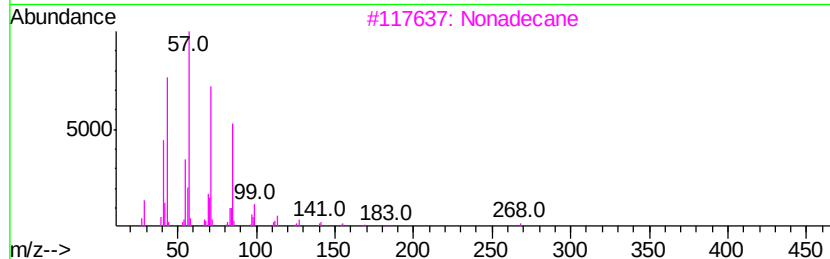
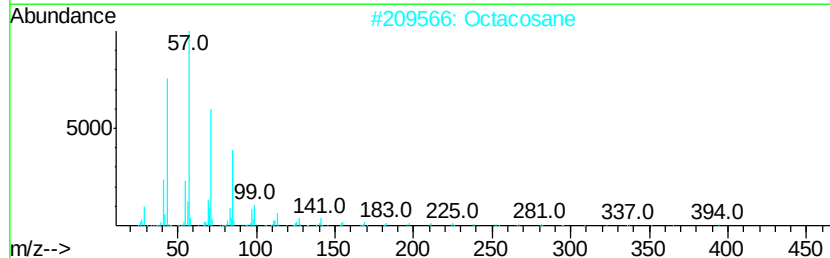
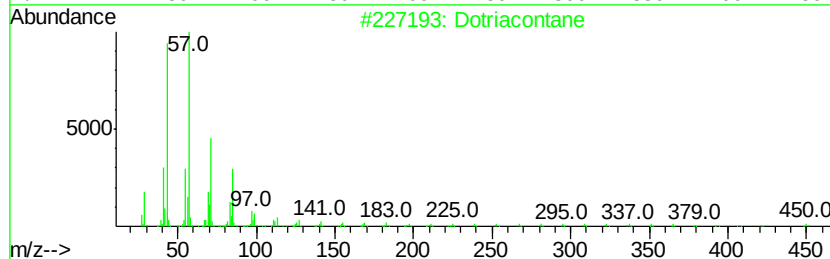
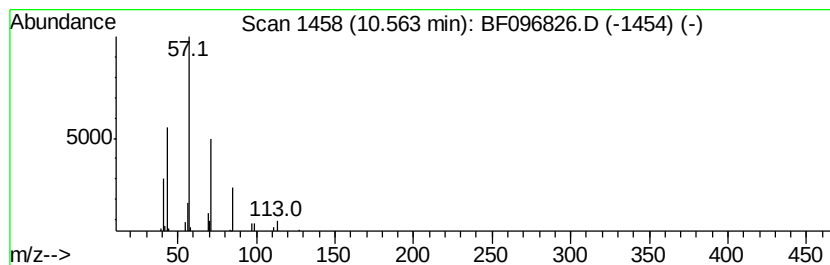
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Dotriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.56	2.70 ng	67425	Phenanthrene-d10	11.11

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dotriacontane	451	C32H66	000544-85-4	90
2		Octacosane	394	C28H58	000630-02-4	86
3		Nonadecane	268	C19H40	000629-92-5	86
4		Hexadecane	226	C16H34	000544-76-3	86
5		Pentadecane	212	C15H32	000629-62-9	80



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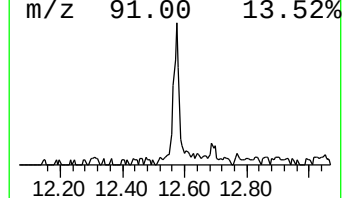
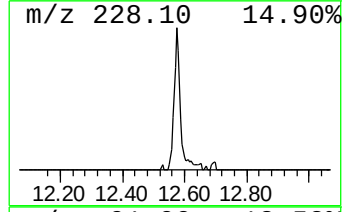
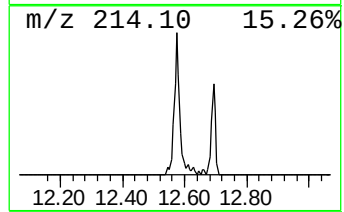
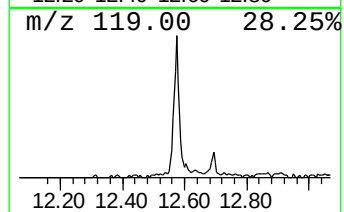
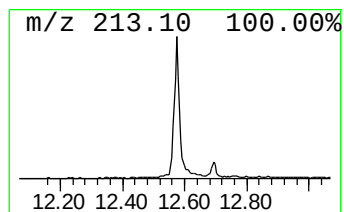
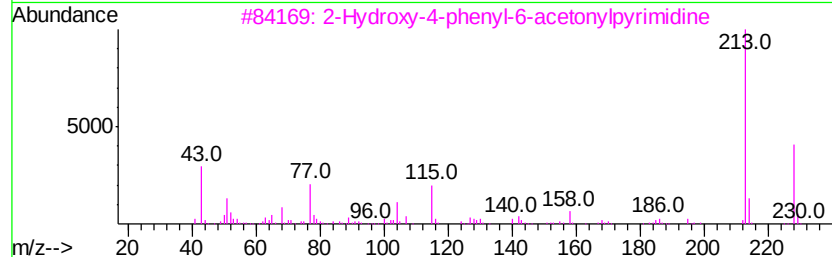
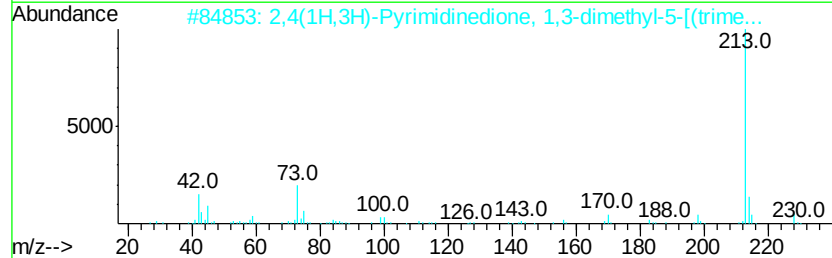
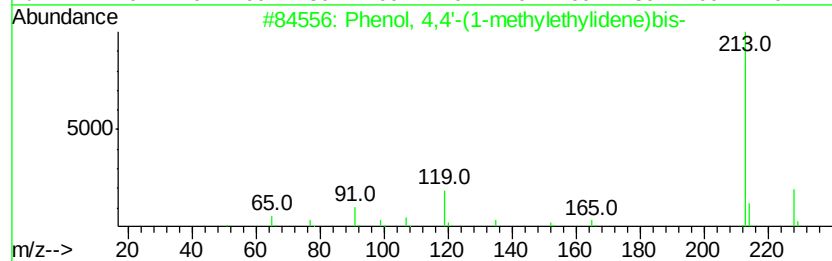
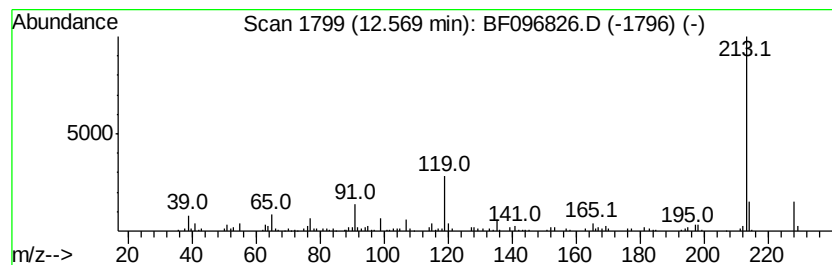
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Phenol, 4,4'-(1-methylethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	9.88 ng	308980	Chrysene-d12	13.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenol, 4,4'-(1-methylethylidene)bis-	228	C15H16O2	000080-05-7	97
2		2,4(1H,3H)-Pyrimidinedione, 1,3-dimethyl-5-[(trimethylsilyl)ethynyl]-	228	C9H16N2O3Si	089447-84-7	53
3		2-Hydroxy-4-phenyl-6-acetylpyrimidine	228	C13H12N2O2	050324-22-6	50
4		1,4-Naphthalenedione, 2-(1-butenyl)-	228	C14H12O3	029366-43-6	47
5		Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	47



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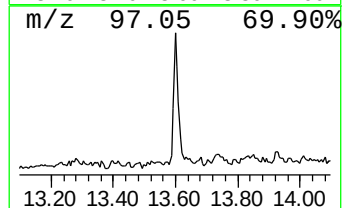
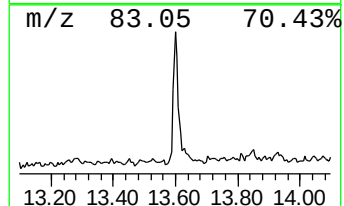
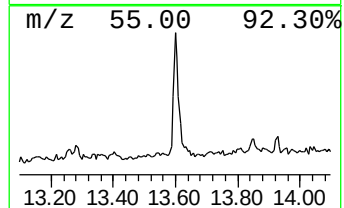
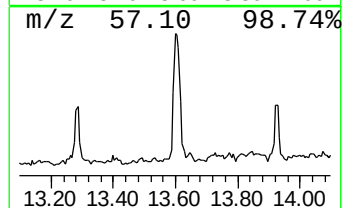
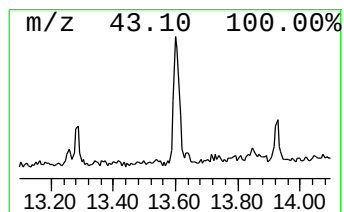
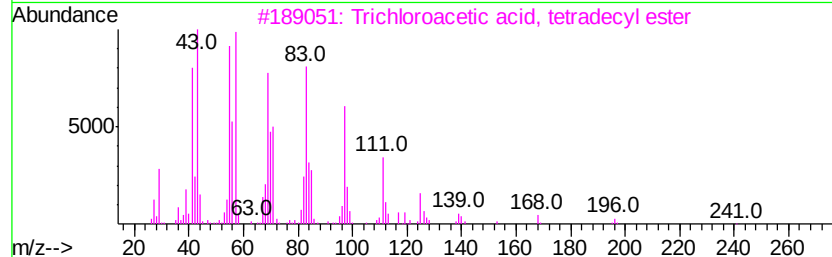
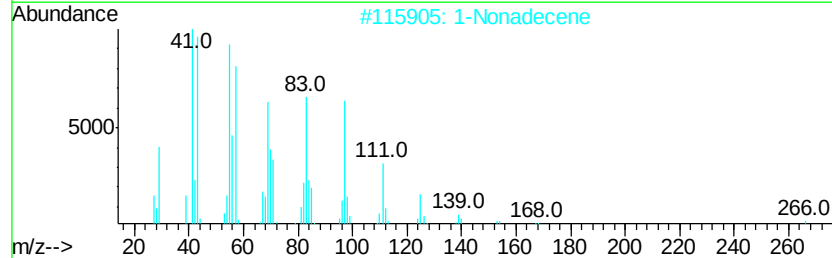
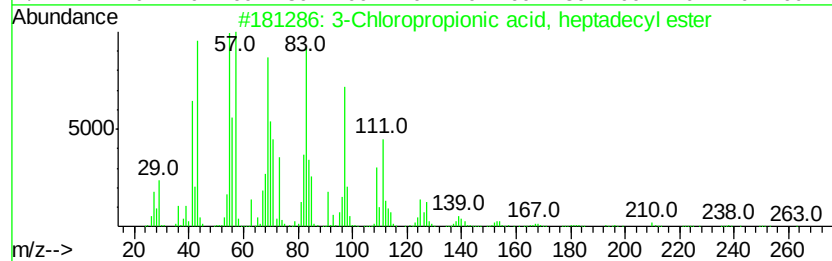
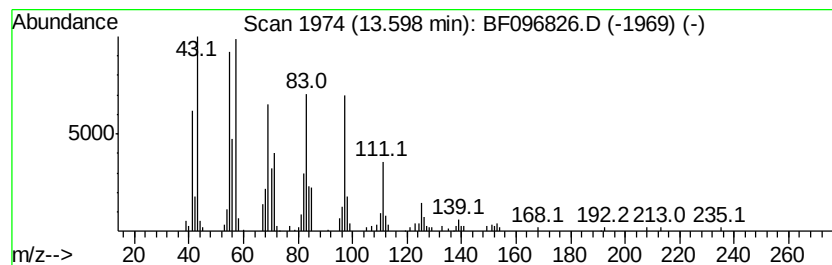
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 3-Chloropropionic acid, hep... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	7.65 ng	239316	Chrysene-d12	13.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
2		1-Nonadecene	266	C19H38	018435-45-5	91
3		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5		1-Docosene	308	C22H44	001599-67-3	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071717\
Data File : BF096826.D
Acq On : 17 Jul 2017 18:23
Operator : SJ/JU
Sample : I4203-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-SB02A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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...	4.78	8.5	ng	235581	1	6.61	554119	20.0
unknown6.38	6.38	77.0	ng	2133190	1	6.61	554119	20.0
Dotriacontane	10.56	2.7	ng	67425	4	11.11	499303	20.0
Phenol, 4,4'-(1-m...	12.57	9.9	ng	308980	5	13.73	625598	20.0
3-Chloropropionic...	13.60	7.7	ng	239316	5	13.73	625598	20.0