

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040919\
 Data File : BF113661.D
 Acq On : 9 Apr 2019 15:08
 Operator : JU/SJ
 Sample : K2316-07
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20190175-AMND-COMP-CS-2

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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	4.863	468	472	487	rBV	210644	317092	9.61%	1.117%
2	5.292	542	545	571	rBV	1841081	2268921	68.74%	7.991%
3	6.334	717	722	738	rBV	2678084	2985336	90.44%	10.514%
4	6.451	738	742	764	rVB	2821386	2724644	82.54%	9.596%
5	6.675	777	780	793	rVB	642228	650925	19.72%	2.293%
6	6.834	803	807	821	rVB	2468431	2215742	67.13%	7.804%
7	7.245	873	877	892	rBV	1830532	1881171	56.99%	6.625%
8	7.963	995	999	1017	rBV	754076	837092	25.36%	2.948%
9	8.639	1111	1114	1117	rVB	57978	42367	1.28%	0.149%
10	9.033	1177	1181	1190	rBV	3322986	3048306	92.35%	10.736%
11	9.427	1245	1248	1258	rBV	331870	337570	10.23%	1.189%
12	9.663	1283	1288	1292	rBV2	21333	37450	1.13%	0.132%
13	9.710	1292	1296	1307	rVB	1055432	978499	29.64%	3.446%
14	10.498	1426	1430	1444	rBV	1741007	1806484	54.73%	6.362%
15	10.610	1446	1449	1452	rBV	76063	63185	1.91%	0.223%
16	11.051	1521	1524	1528	rBV2	25153	34578	1.05%	0.122%
17	11.192	1544	1548	1556	rBV	1124637	1068959	32.38%	3.765%
18	11.727	1636	1639	1649	rBV2	256878	305882	9.27%	1.077%
19	12.510	1770	1772	1779	rBV	40306	58082	1.76%	0.205%
20	12.651	1790	1796	1798	rBV2	26320	40809	1.24%	0.144%
21	12.774	1812	1817	1820	rBV	3519436	3300901	100.00%	11.626%
22	13.345	1909	1914	1917	rBV2	33958	37322	1.13%	0.131%
23	13.674	1967	1970	1974	rVB	46609	41292	1.25%	0.145%
24	13.804	1987	1992	1993	rBV	207202	207334	6.28%	0.730%
25	13.827	1993	1996	2019	rVV	1137391	1542730	46.74%	5.434%
26	13.986	2020	2023	2030	rVB	70269	74306	2.25%	0.262%
27	14.292	2069	2075	2079	rBV	95176	103750	3.14%	0.365%
28	14.586	2121	2125	2131	rVB	112246	115399	3.50%	0.406%
29	14.651	2133	2136	2139	rVB	92184	80784	2.45%	0.285%
30	14.892	2174	2177	2182	rVB	119682	125690	3.81%	0.443%
31	15.233	2230	2235	2248	rVB	709346	952927	28.87%	3.356%
32	15.633	2299	2303	2310	rVB	73117	107375	3.25%	0.378%

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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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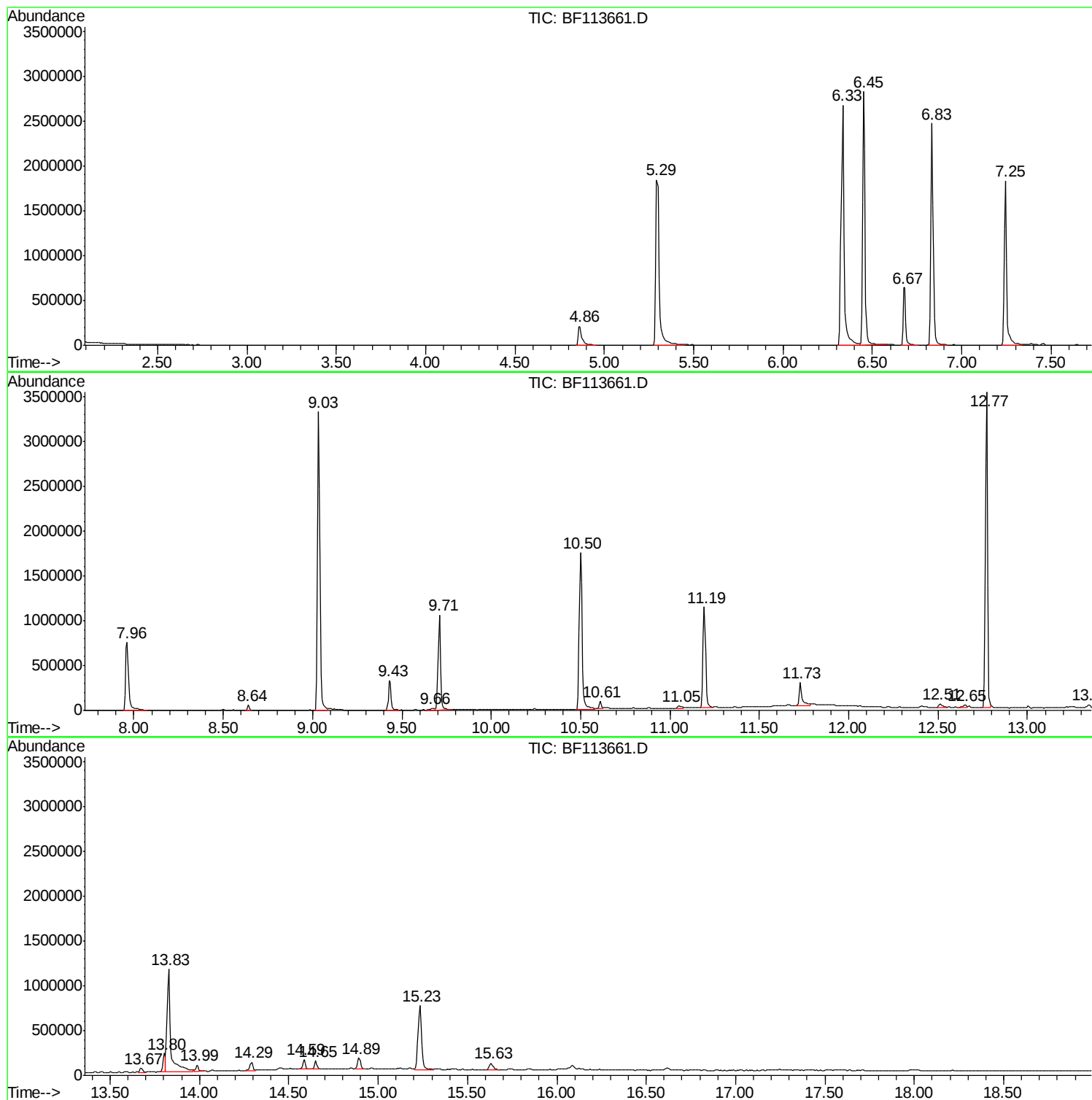
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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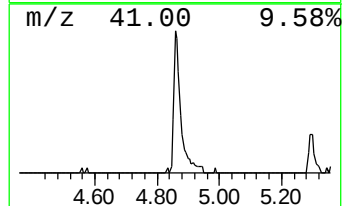
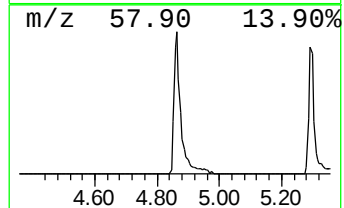
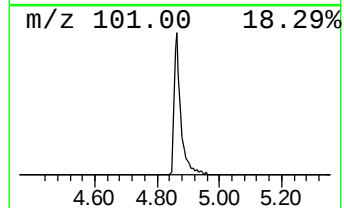
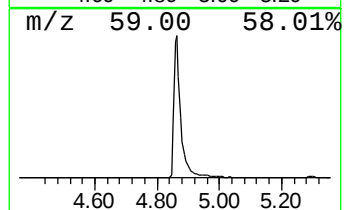
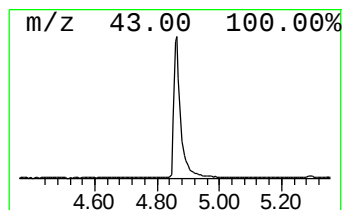
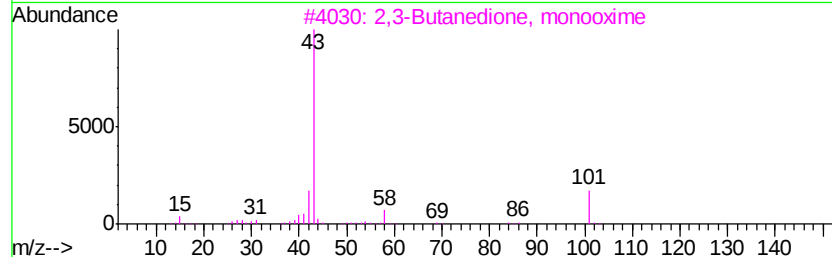
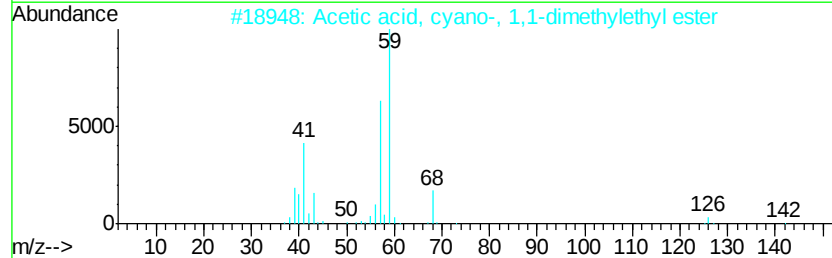
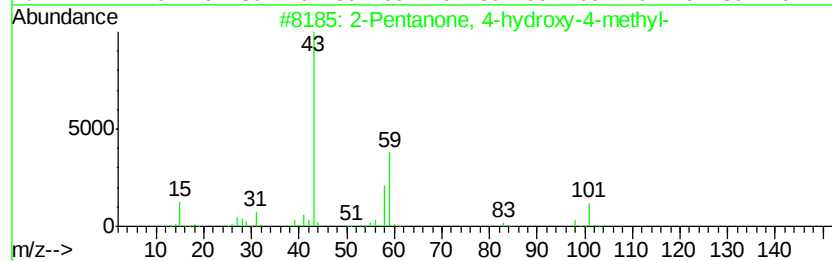
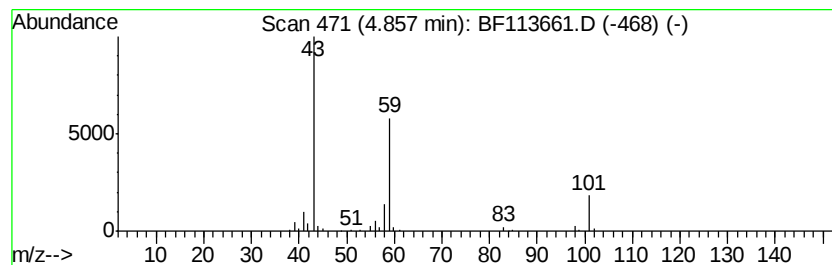
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	9.74 ng	317092	1,4-Dichlorobenzene-d4	6.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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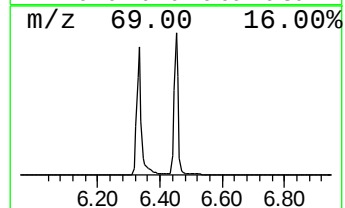
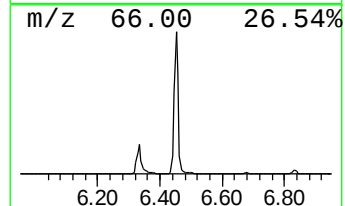
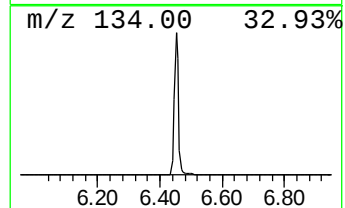
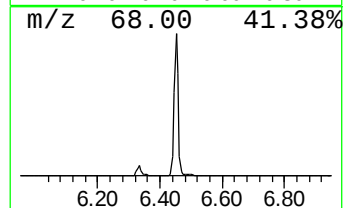
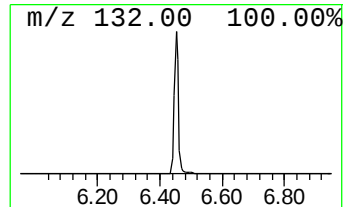
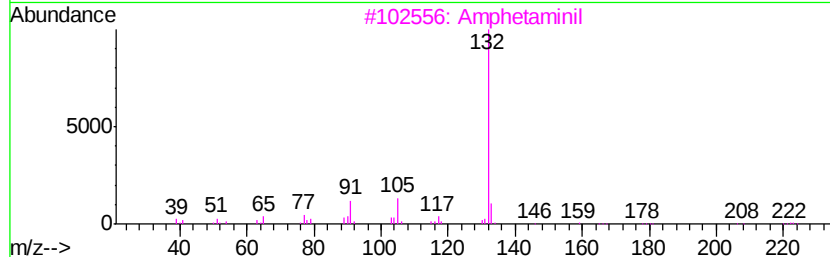
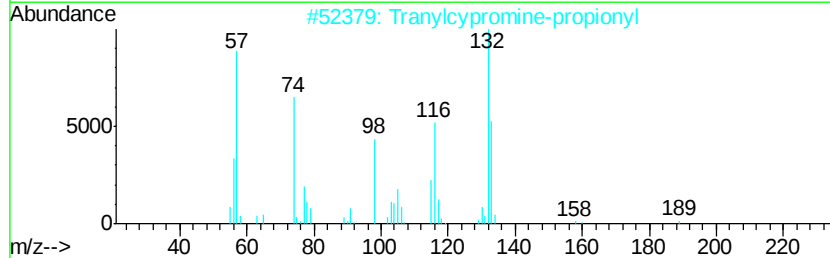
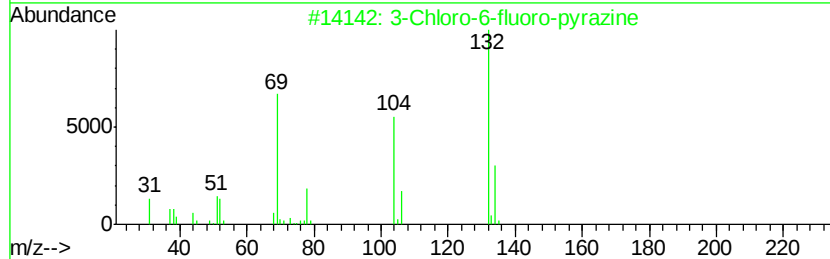
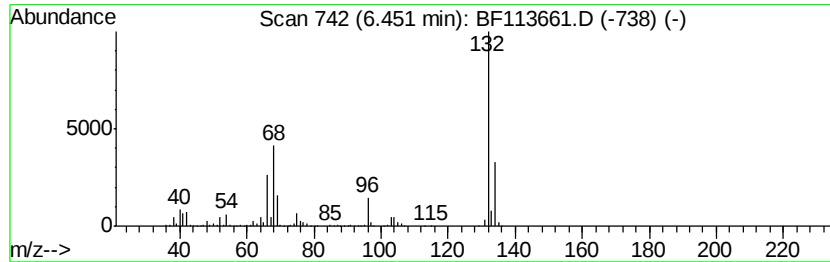
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	83.72 ng	2724640	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		Amphetaminil	250	C17H18N2	017590-01-1	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12



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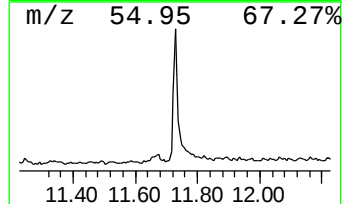
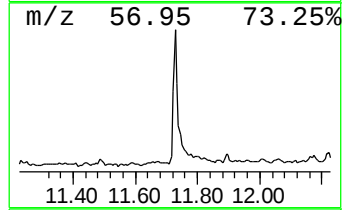
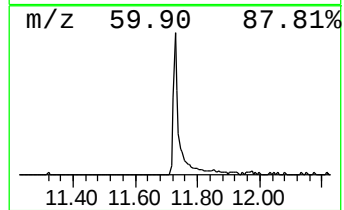
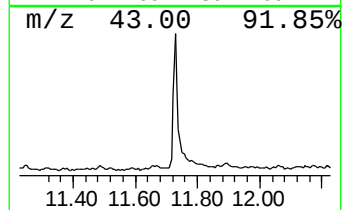
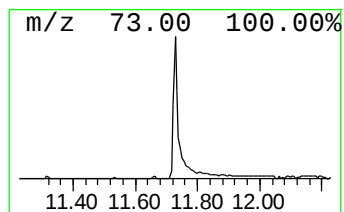
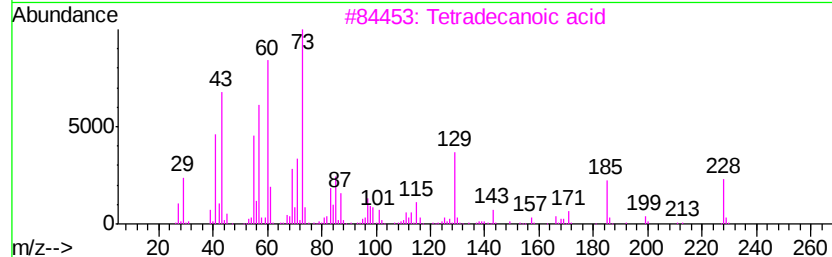
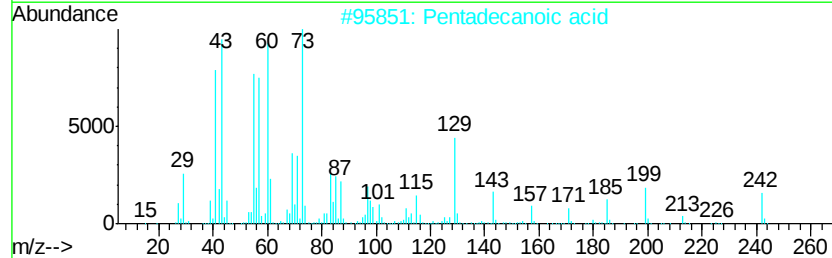
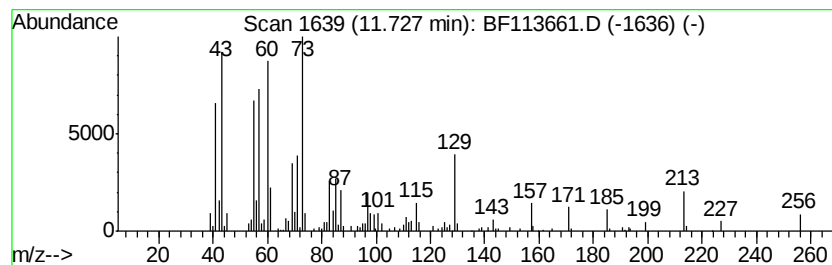
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.73	5.72 ng	305882	Phenanthrene-d10	11.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4		n-Decanoic acid	172	C10H20O2	000334-48-5	68
5		Tridecanoic acid	214	C13H26O2	000638-53-9	64



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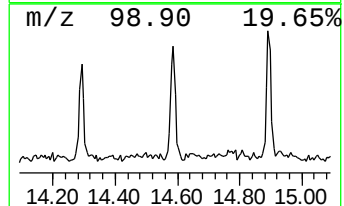
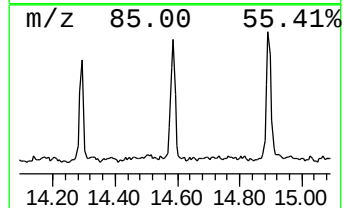
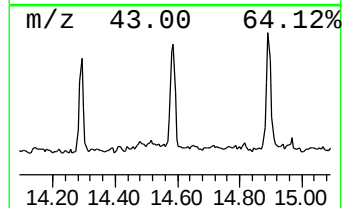
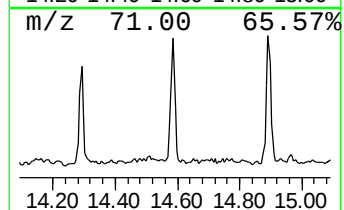
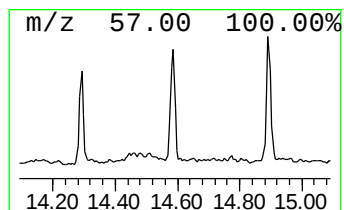
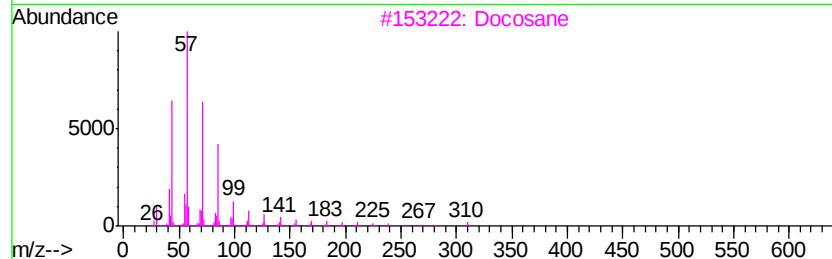
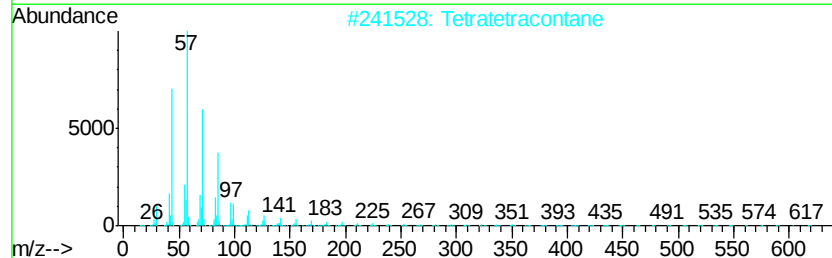
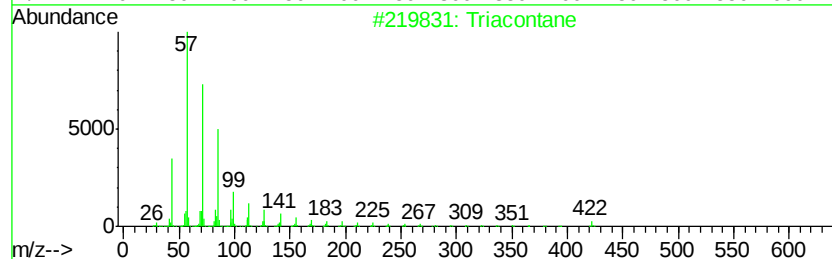
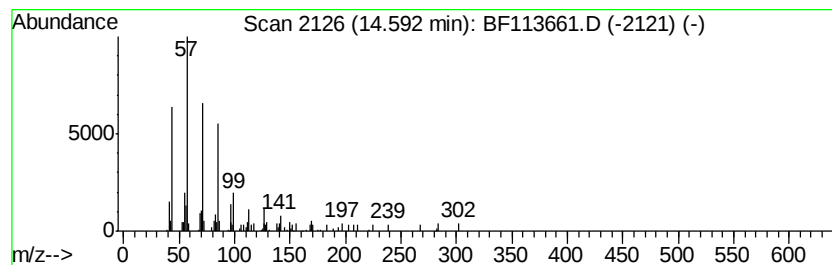
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Triacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	2.42 ng	115399	Perylene-d12	15.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triacontane	422	C30H62	000638-68-6	91
2		Tetratetracontane	619	C44H90	007098-22-8	91
3		Docosane	310	C22H46	000629-97-0	90
4		Tetracosane	338	C24H50	000646-31-1	87
5		Octadecane	254	C18H38	000593-45-3	87



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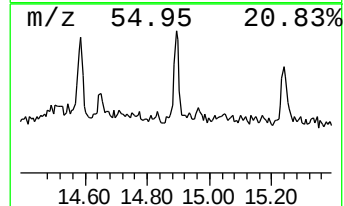
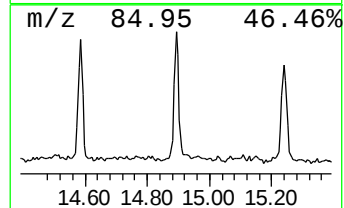
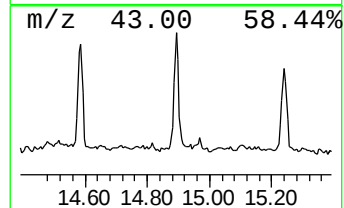
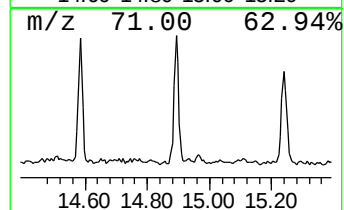
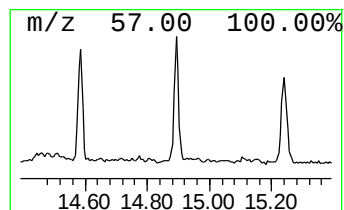
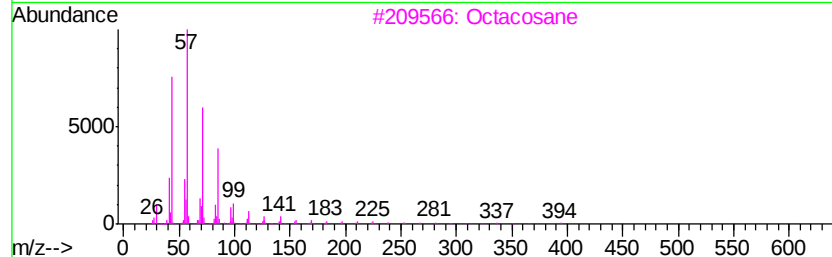
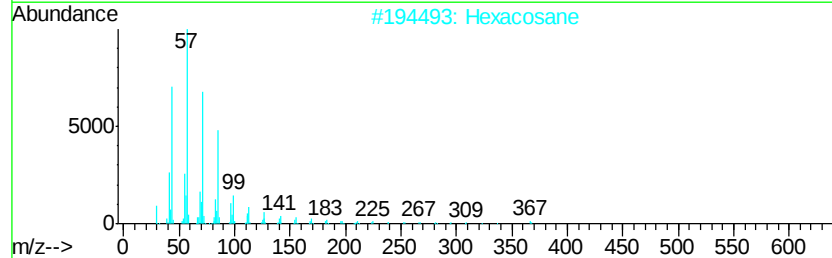
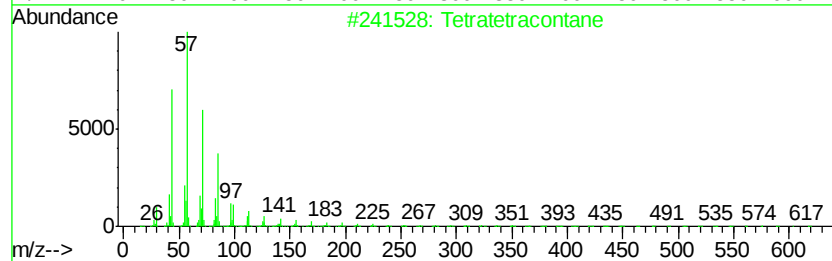
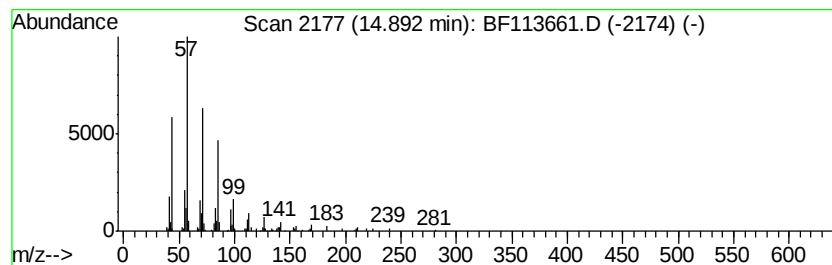
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tetratetracontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	2.64 ng	125690	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Hentriacontane	437	C31H64	000630-04-6	91
5		Tetracosane	338	C24H50	000646-31-1	91



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20190175-AMND-COMP-CS-2

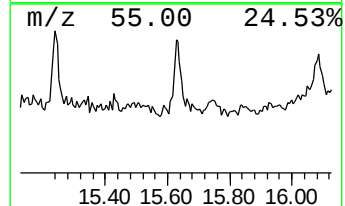
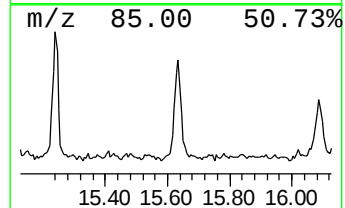
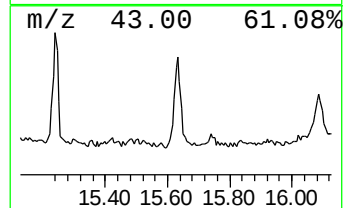
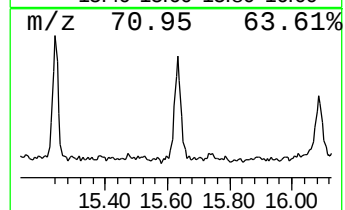
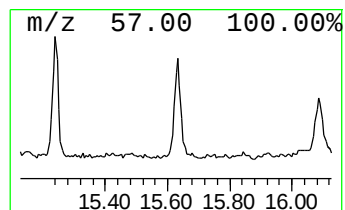
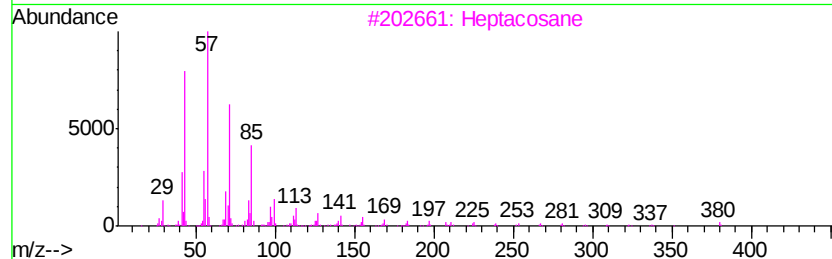
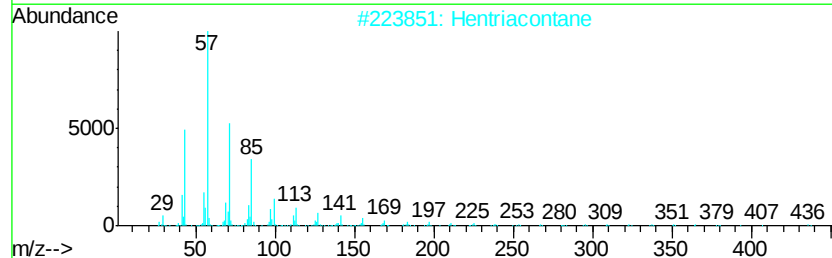
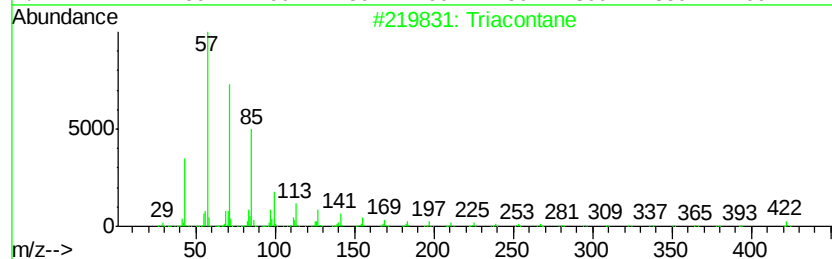
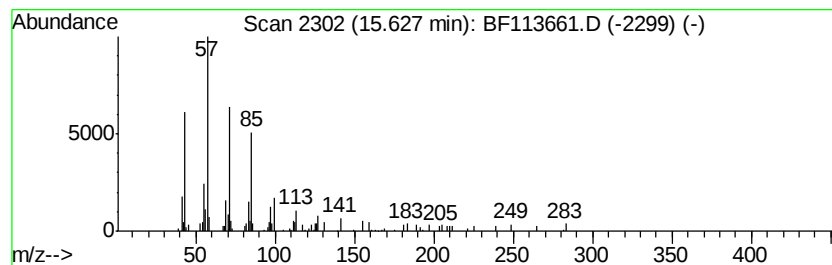
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.63	2.25 ng	107375	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	90
2		Hentriacontane	437	C31H64	000630-04-6	90
3		Heptacosane	380	C27H56	000593-49-7	87
4		2-methyloctacosane	408	C29H60	1000376-72-8	87
5		Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040919\
Data File : BF113661.D
Acq On : 9 Apr 2019 15:08
Operator : JU/SJ
Sample : K2316-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20190175-AMND-COMP-CS-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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...	4.86	9.7	ng	317092	1	6.68	650925	20.0
unknown6.45	6.45	83.7	ng	2724640	1	6.68	650925	20.0
n-Hexadecanoic acid	11.73	5.7	ng	305882	4	11.19	1068960	20.0
Triacontane	14.59	2.4	ng	115399	6	15.23	952927	20.0
Tetratetracontane	14.89	2.6	ng	125690	6	15.23	952927	20.0
Hentriacontane	15.63	2.3	ng	107375	6	15.23	952927	20.0