

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
 Data File : BF097156.D
 Acq On : 28 Jul 2017 16:01
 Operator : SJ/JU
 Sample : I4420-06
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 2A-1-2-3-4-5-COMP-(0-10)

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	463	467	482	rVB	166014	280239	9.81%	1.253%
2	5.087	540	544	562	rBV	2500518	2831567	99.08%	12.660%
3	6.157	721	726	740	rBV	2442044	2857744	100.00%	12.778%
4	6.263	740	744	747	rBV	2762943	2635522	92.22%	11.784%
5	6.486	778	782	791	rBV	769265	651557	22.80%	2.913%
6	6.645	804	809	812	rBV	2096045	1990001	69.64%	8.898%
7	7.057	874	879	882	rBV	1756463	1609053	56.31%	7.194%
8	7.769	996	1000	1004	rBV	1036150	857407	30.00%	3.834%
9	8.851	1179	1184	1187	rBV	2417314	2277669	79.70%	10.184%
10	9.245	1247	1251	1257	rBV	270932	211445	7.40%	0.945%
11	9.516	1293	1297	1301	rBV	844082	755766	26.45%	3.379%
12	9.969	1371	1374	1377	rVB	47435	37078	1.30%	0.166%
13	10.298	1427	1430	1437	rBV	1145515	1113498	38.96%	4.979%
14	10.439	1452	1454	1460	rVB	60773	59801	2.09%	0.267%
15	10.886	1527	1530	1532	rVB	38890	31123	1.09%	0.139%
16	10.986	1543	1547	1550	rBV	708415	595173	20.83%	2.661%
17	11.010	1550	1551	1556	rVB	52521	35575	1.24%	0.159%
18	11.545	1639	1642	1649	rBV2	91925	87940	3.08%	0.393%
19	12.192	1749	1752	1756	rVB	86415	72732	2.55%	0.325%
20	12.327	1769	1775	1782	rBV3	37749	60786	2.13%	0.272%
21	12.416	1786	1790	1794	rVB	77398	80571	2.82%	0.360%
22	12.574	1812	1817	1820	rVB	1515035	1465314	51.28%	6.552%
23	13.486	1965	1972	1978	rBV2	106026	151444	5.30%	0.677%
24	13.610	1989	1993	1996	rBV	654238	646252	22.61%	2.890%
25	13.639	1996	1998	2003	rVB	40715	38761	1.36%	0.173%
26	14.115	2075	2079	2086	rVB6	22027	46101	1.61%	0.206%
27	14.604	2159	2162	2169	rBV	56165	112466	3.94%	0.503%
28	14.692	2175	2177	2185	rVB7	24951	32591	1.14%	0.146%
29	14.857	2203	2205	2209	rVB2	27024	30492	1.07%	0.136%
30	14.909	2211	2214	2218	rVB	27220	33876	1.19%	0.151%
31	14.962	2218	2223	2228	rBV	450027	543320	19.01%	2.429%
32	15.009	2228	2231	2236	rVB6	23910	35745	1.25%	0.160%
33	15.368	2288	2292	2295	rVB4	22237	32867	1.15%	0.147%
34	17.862	2711	2716	2717	rBV5	18502	31100	1.09%	0.139%

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2A-1-2-3-4-5-COMP-(0-10)

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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35	19.127	2926	2931	2933	rBV4	18454	32792	1.15%	0.147%
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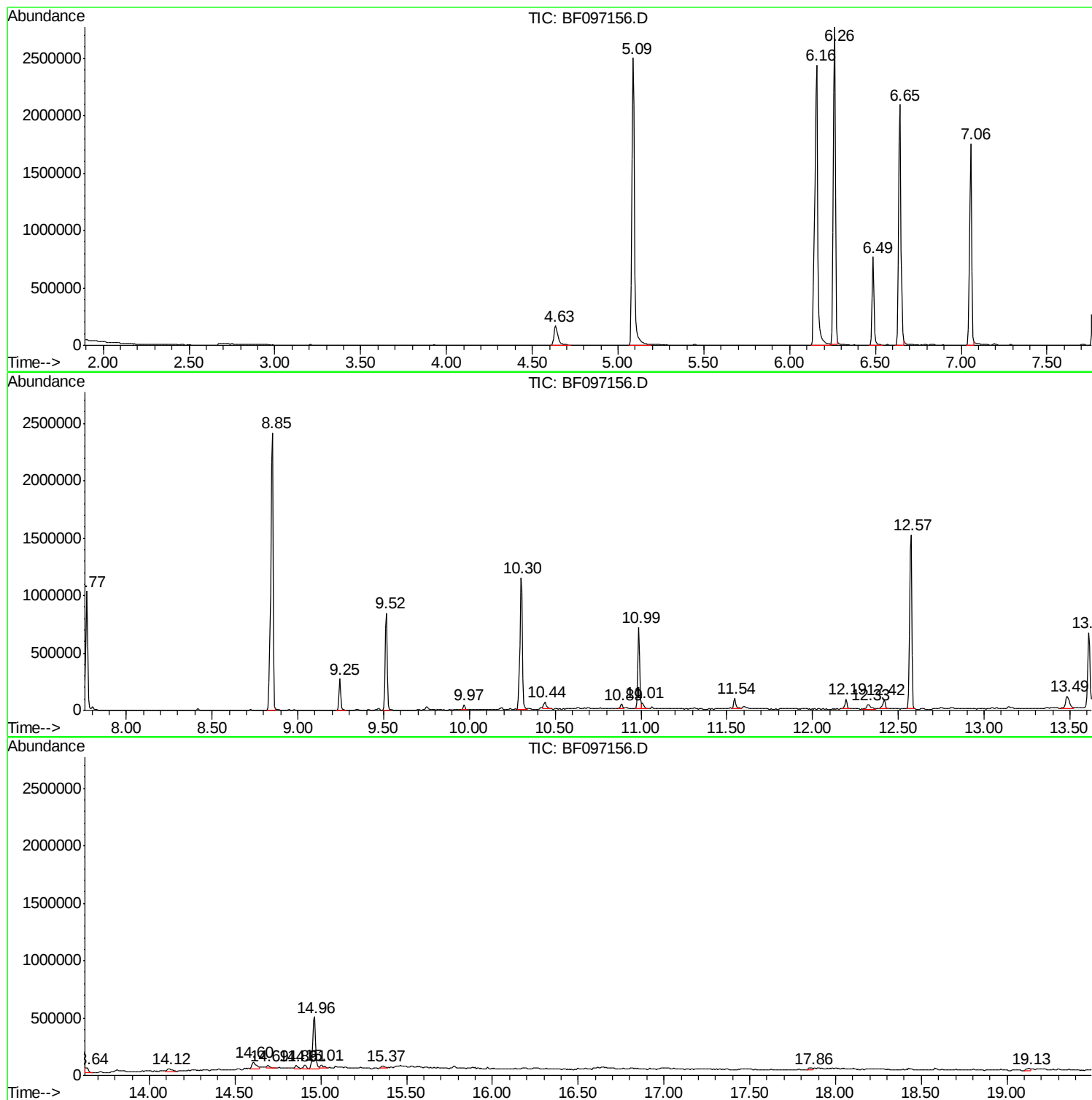
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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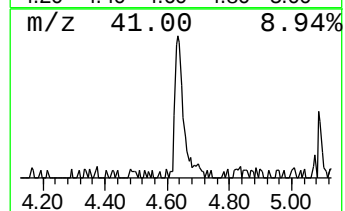
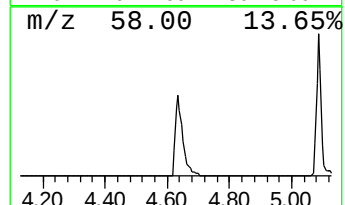
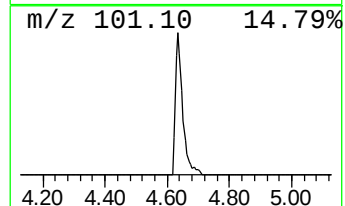
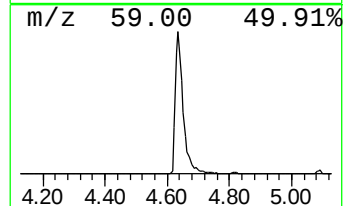
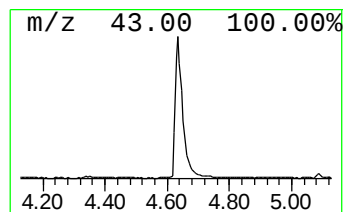
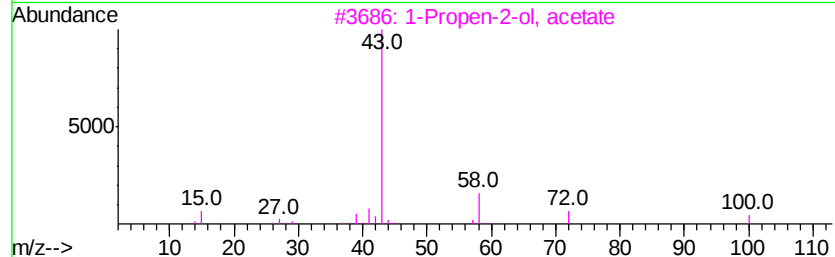
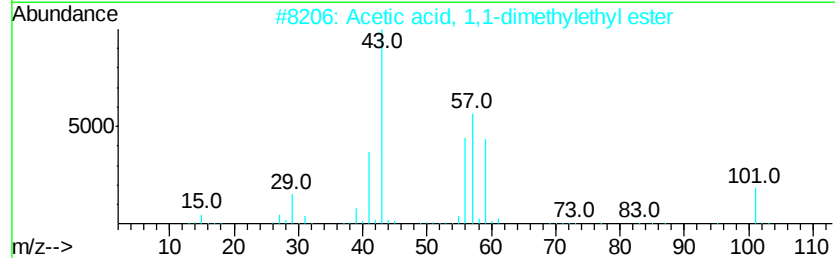
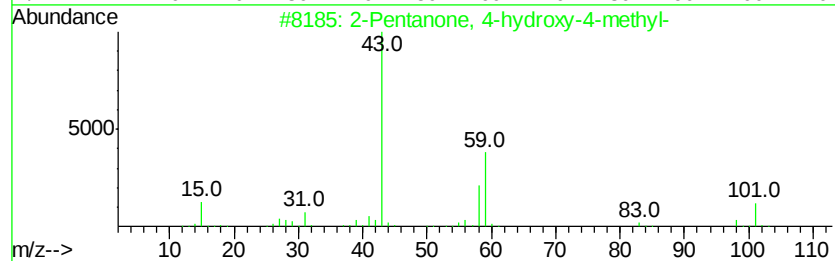
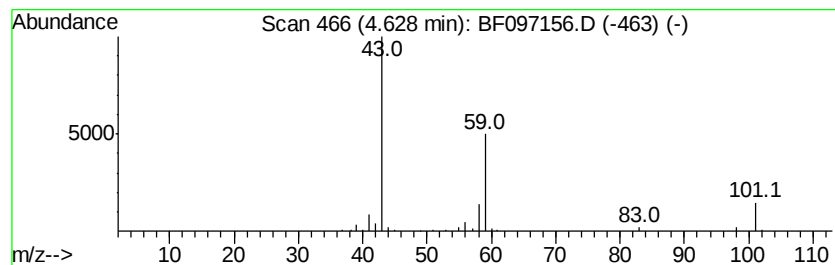
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	8.60 ng	280239	1,4-Dichlorobenzene-d4	6.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4			5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9
5			Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7



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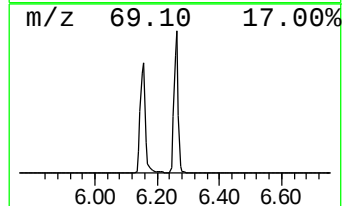
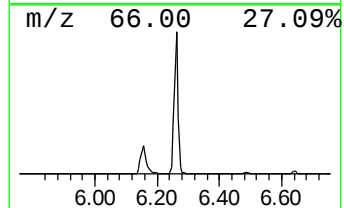
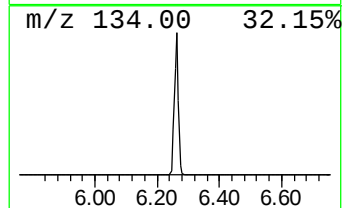
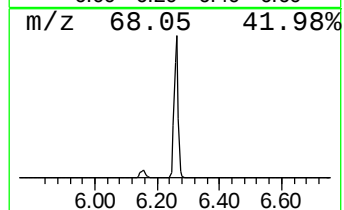
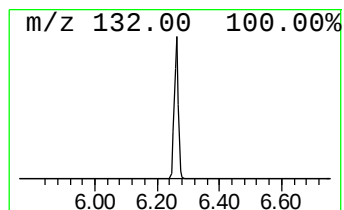
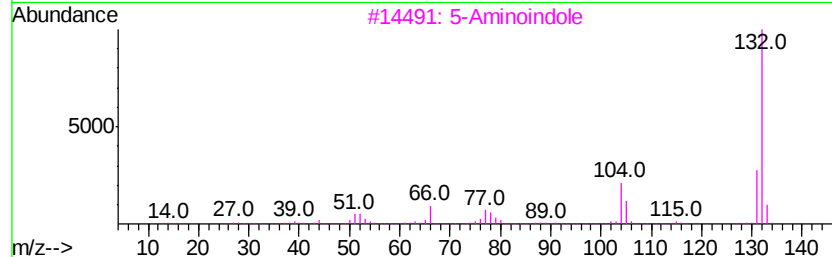
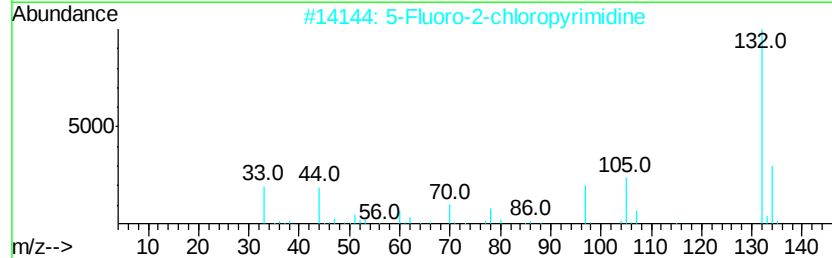
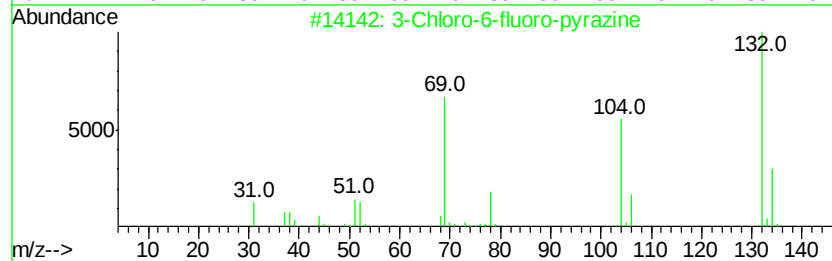
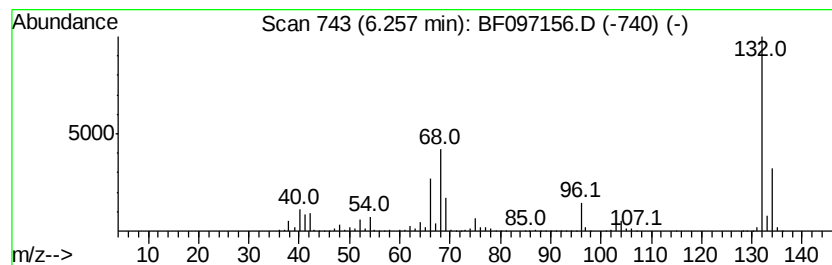
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	80.90 ng	2635520	1,4-Dichlorobenzene-d4	6.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3	Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5	Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5	Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranvlcvpromine-propionvl	189	C12H15NO	1000123-86-3	10	
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9	



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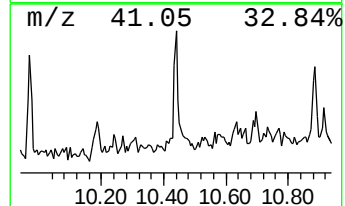
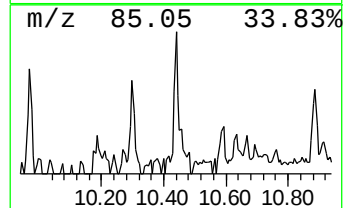
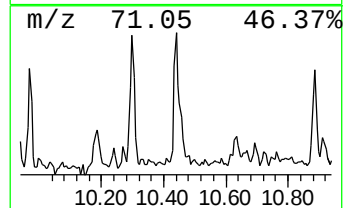
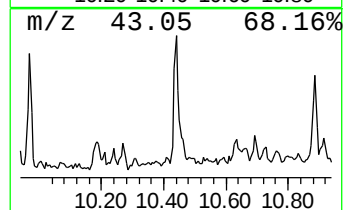
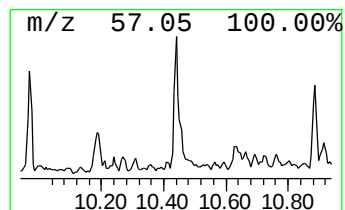
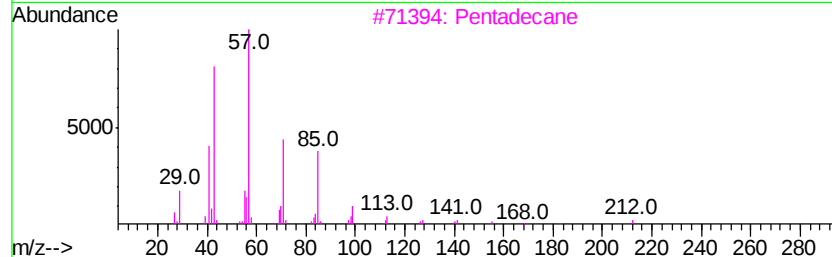
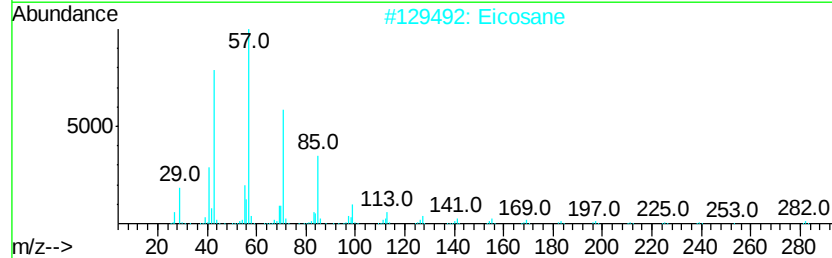
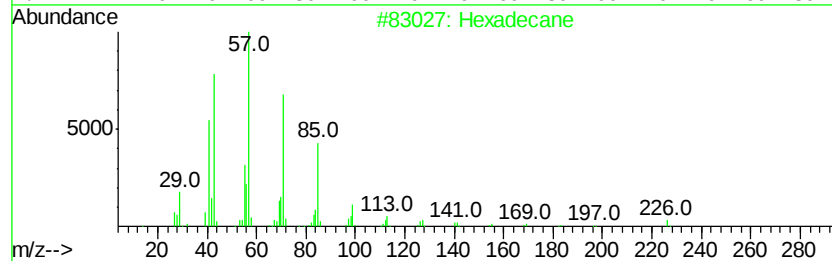
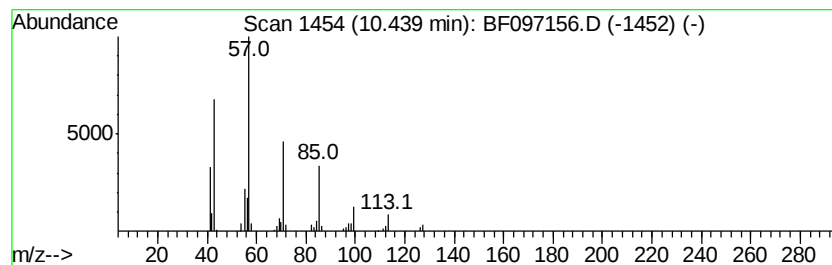
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.44	2.01 ng	59801	Phenanthrene-d10		10.99
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Eicosane	282	C20H42	000112-95-8	78
3	Pentadecane	212	C15H32	000629-62-9	78
4	Tridecane	184	C13H28	000629-50-5	72
5	Nonadecane	268	C19H40	000629-92-5	72



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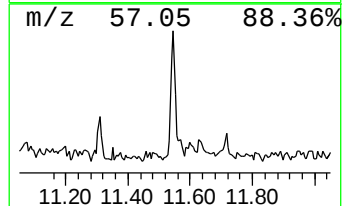
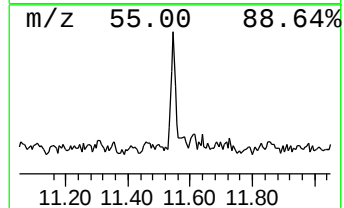
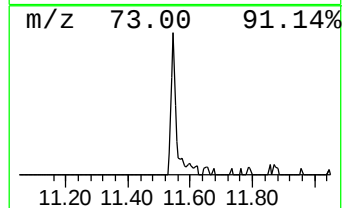
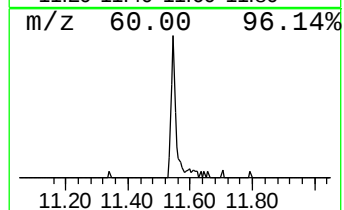
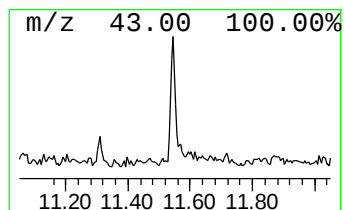
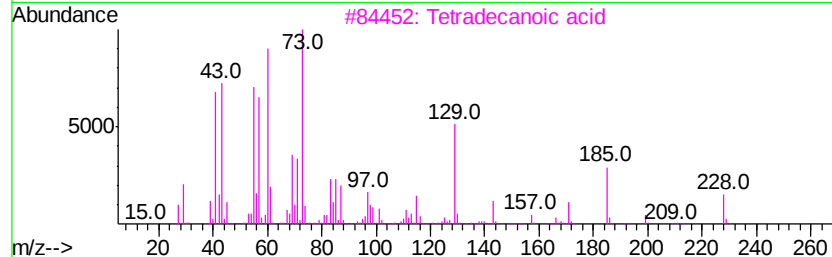
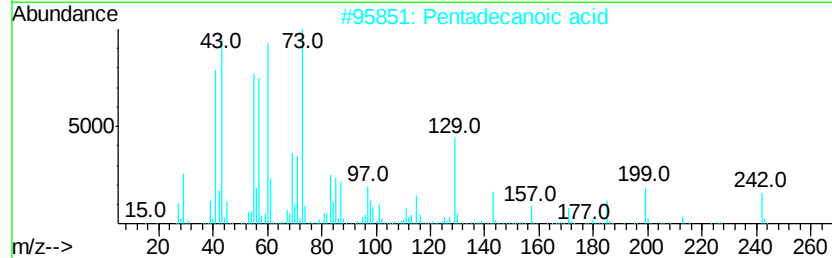
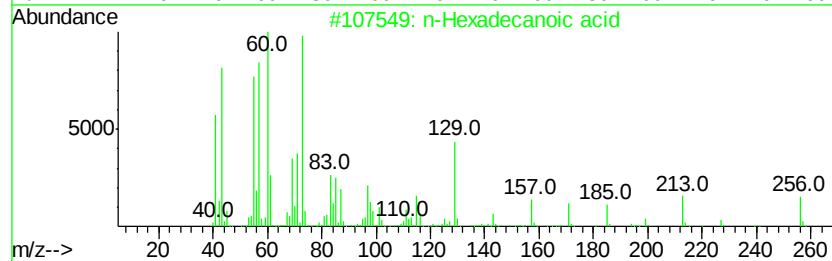
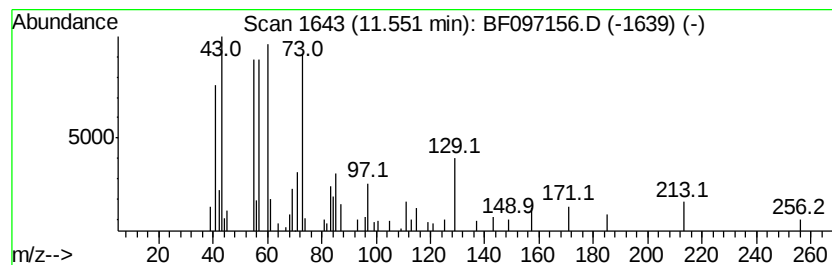
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	2.96 ng	87940	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58



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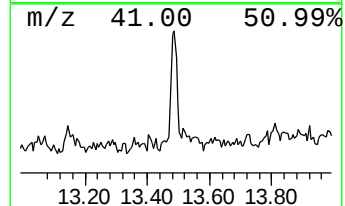
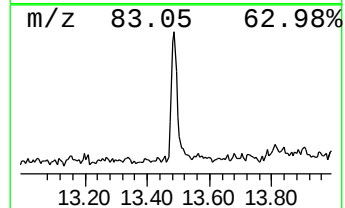
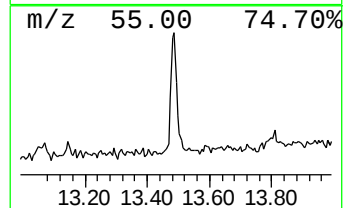
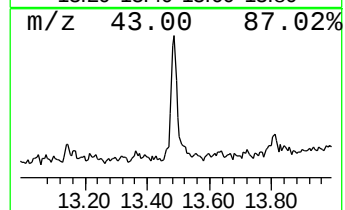
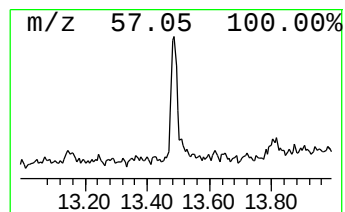
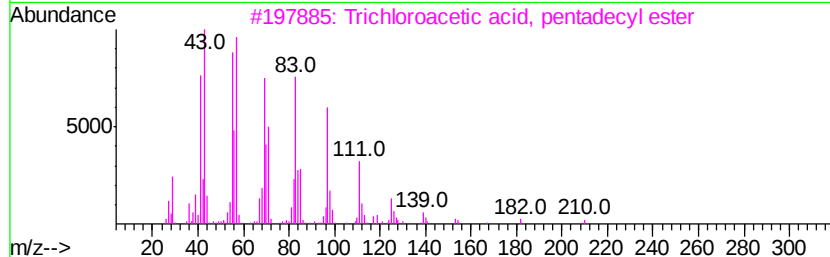
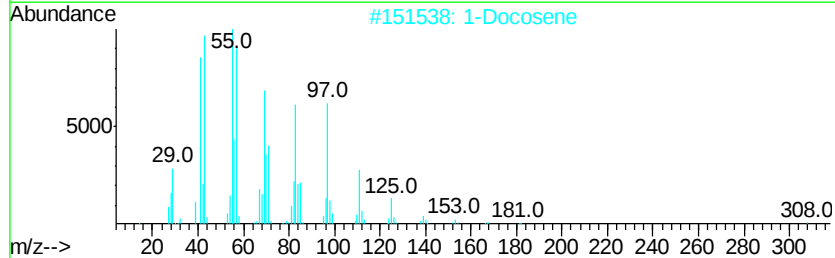
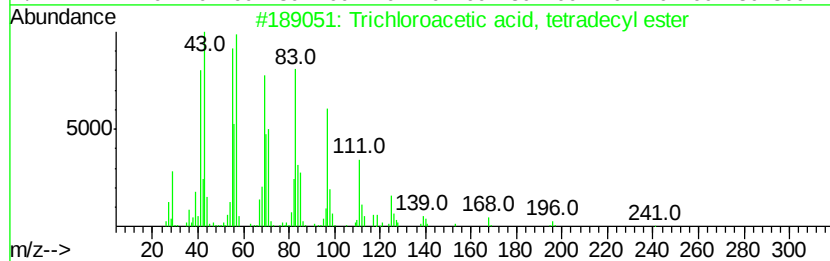
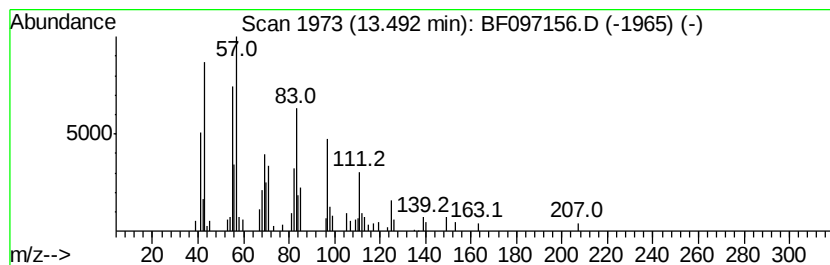
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Peak Number 7 Trichloroacetic acid, tetra... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.49	4.69 ng	151444	Chrysene-d12	13.61	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	94
2	1-Docosene	308	C22H44	001599-67-3	94
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	91
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072817\
Data File : BF097156.D
Acq On : 28 Jul 2017 16:01
Operator : SJ/JU
Sample : I4420-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2A-1-2-3-4-5-COMP-(0-10)

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	8.6	ng	280239	1	6.49	651557	20.0
unknown6.26	6.26	80.9	ng	2635520	1	6.49	651557	20.0
Hexadecane	10.44	2.0	ng	59801	4	10.99	595173	20.0
n-Hexadecanoic acid	11.55	3.0	ng	87940	4	10.99	595173	20.0
Trichloroacetic a...	13.49	4.7	ng	151444	5	13.61	646252	20.0