

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100917\
 Data File : BF099268.D
 Acq On : 9 Oct 2017 17:56
 Operator : SJ/JU
 Sample : I5651-11
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ENV-116-7(0-5)

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	2.163	9	13	18	rVB	33863	42584	1.49%	0.179%
2	5.092	508	511	527	rVB	370320	477808	16.76%	2.013%
3	5.492	574	579	582	rBV	2418648	2355689	82.65%	9.925%
4	6.498	745	750	753	rBV	2273201	2396878	84.09%	10.098%
5	6.633	769	773	777	rBV	2544738	2509647	88.05%	10.573%
6	6.863	808	812	816	rBV	854113	679727	23.85%	2.864%
7	7.022	834	839	842	rBV	2120876	1953963	68.55%	8.232%
8	7.428	903	908	911	rBV	1612636	1561636	54.79%	6.579%
9	8.145	1026	1030	1033	rBV	1146417	932258	32.71%	3.928%
10	9.222	1207	1213	1216	rBV	2984559	2850339	100.00%	12.009%
11	9.610	1275	1279	1288	rBV	543402	434855	15.26%	1.832%
12	9.898	1324	1328	1332	rBV2	1202521	1024305	35.94%	4.315%
13	10.316	1397	1399	1403	rVB2	44704	38784	1.36%	0.163%
14	10.692	1458	1463	1466	rBV	1699495	1581561	55.49%	6.663%
15	10.792	1476	1480	1490	rVB	63137	66510	2.33%	0.280%
16	11.386	1577	1581	1584	rBV	1202193	1007595	35.35%	4.245%
17	12.968	1846	1850	1854	rBV	2449255	2357350	82.70%	9.932%
18	13.439	1926	1930	1934	rVB2	40819	37119	1.30%	0.156%
19	13.857	1997	2001	2011	rVB2	71936	96083	3.37%	0.405%
20	14.027	2026	2030	2033	rBV	785495	695819	24.41%	2.932%
21	15.503	2275	2281	2294	rVB	474916	635058	22.28%	2.676%

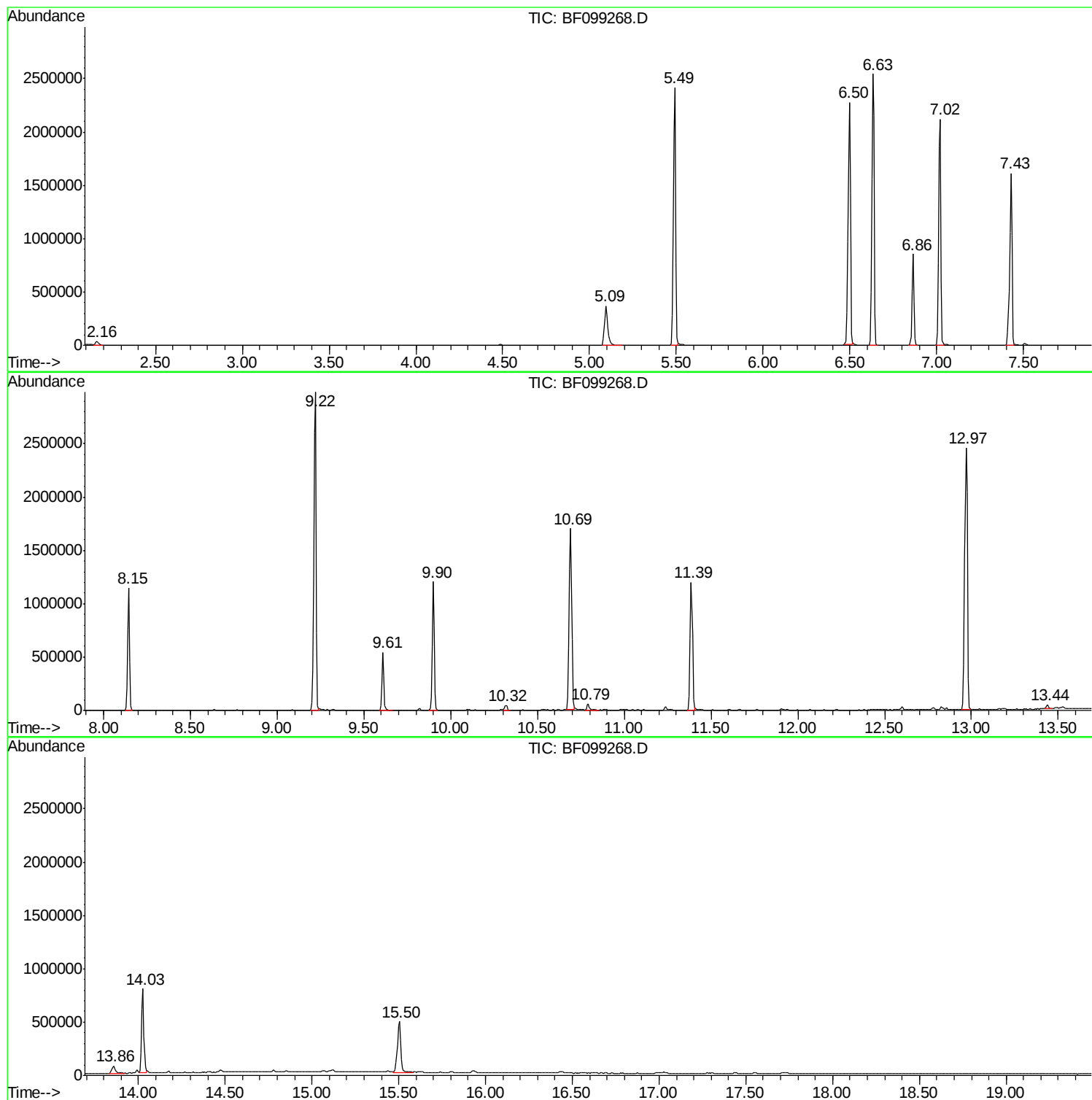
Sum of corrected areas: 23735568

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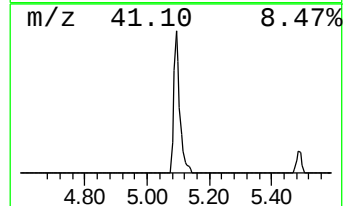
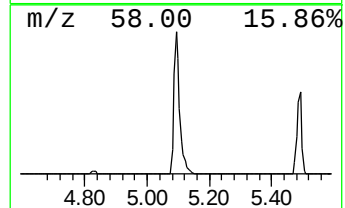
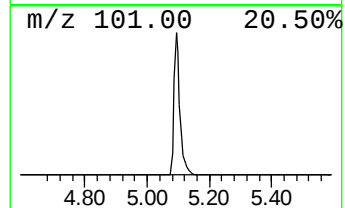
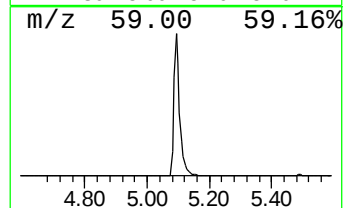
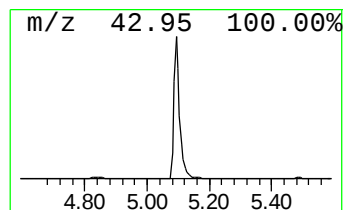
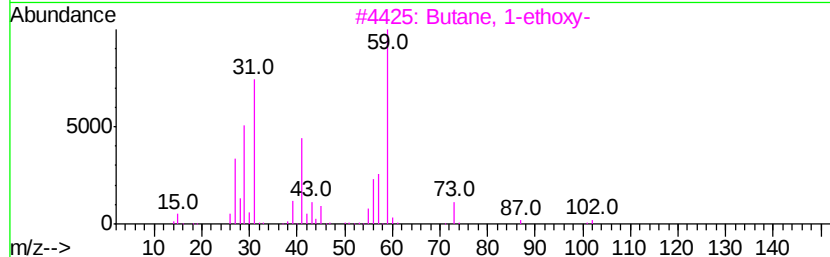
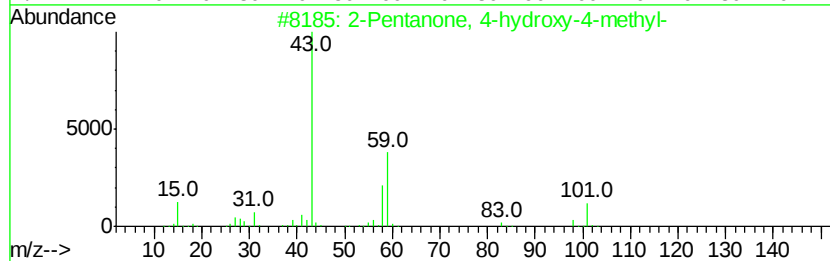
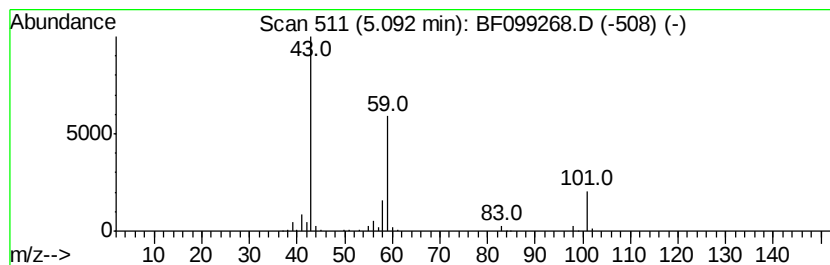
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	14.06 ng	477808	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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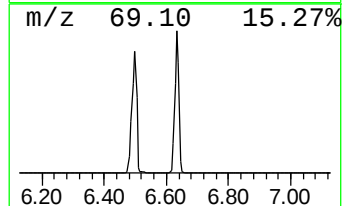
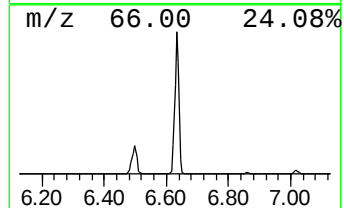
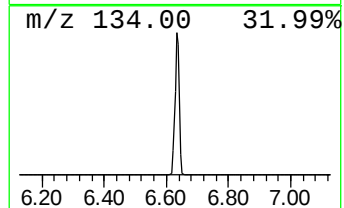
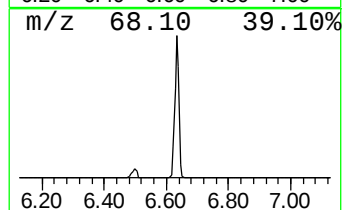
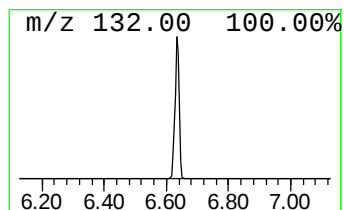
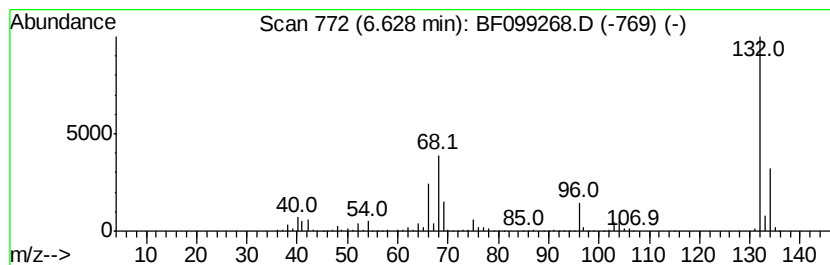
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Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	73.84 ng	2509650	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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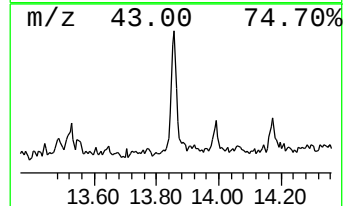
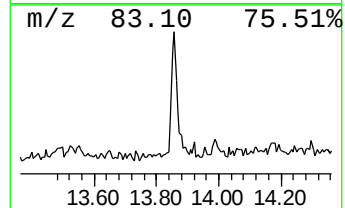
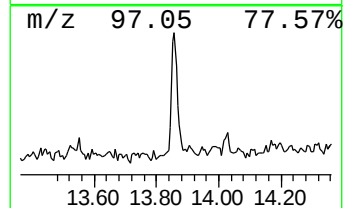
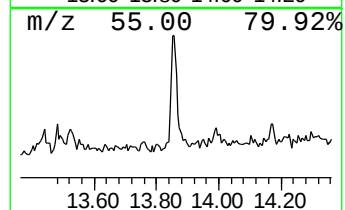
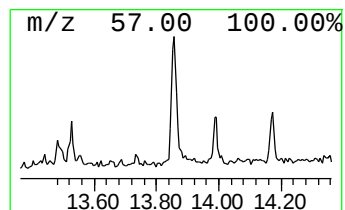
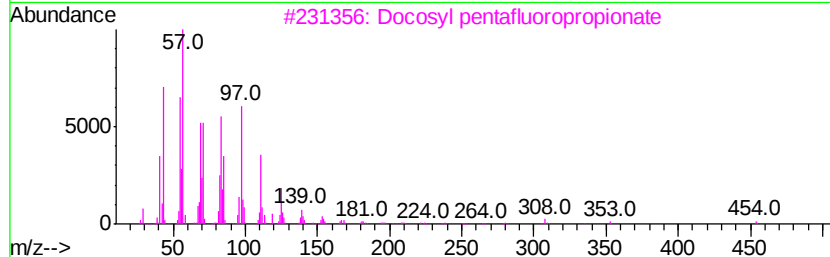
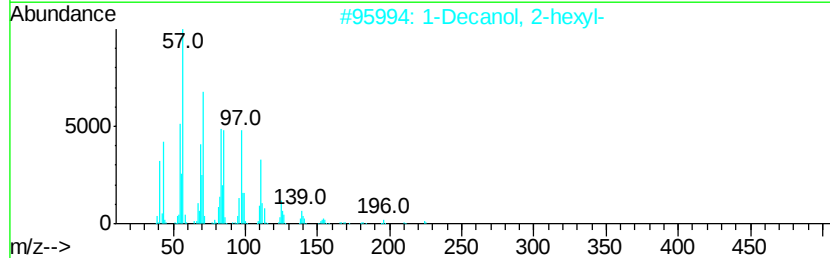
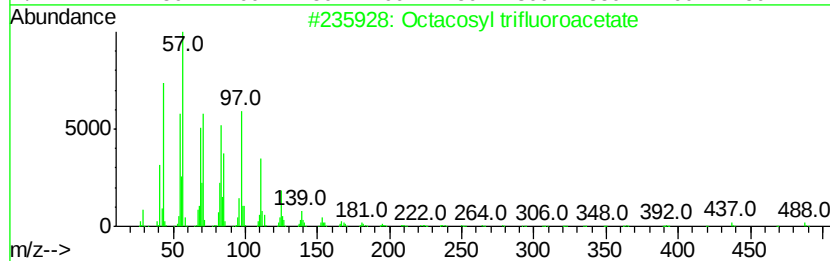
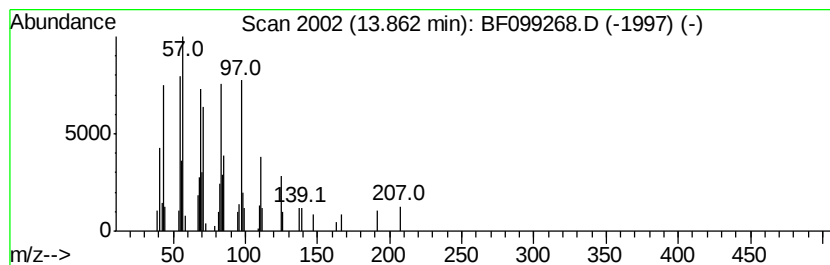
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Peak Number 4 Octacosyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	2.76 ng	96083	Chrysene-d12	14.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	94
2		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
3		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
4		Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	90
5		Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.09	14.1	ng	477808	1	6.86	679727	20.0
unknown6.63	6.63	73.8	ng	2509650	1	6.86	679727	20.0
Octacosyl trifluo...	13.86	2.8	ng	96083	5	14.03	695819	20.0