

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
 Data File : BF099087.D
 Acq On : 5 Oct 2017 00:44
 Operator : SJ/JU
 Sample : I5589-01
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SASP2P-TP-106-T(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	2.169	9	14	21	rVB	178779	236051	5.61%	0.659%
2	5.098	508	512	525	rVB	531772	792637	18.82%	2.212%
3	5.493	573	579	582	rBV	3341051	3661687	86.96%	10.219%
4	6.498	741	750	753	rBV	3000612	3880047	92.14%	10.828%
5	6.640	768	774	777	rBV	3478980	3731037	88.60%	10.412%
6	6.863	808	812	816	rBV	1094943	896762	21.30%	2.503%
7	6.992	831	834	835	rBV	60071	45155	1.07%	0.126%
8	7.022	835	839	842	rVB	3063629	2825899	67.11%	7.886%
9	7.428	902	908	911	rBV	2085822	2424404	57.57%	6.766%
10	8.145	1025	1030	1033	rBV	1373319	1145764	27.21%	3.197%
11	9.222	1207	1213	1216	rBV	4037110	4211010	100.00%	11.752%
12	9.610	1275	1279	1282	rBV	728700	623580	14.81%	1.740%
13	9.898	1324	1328	1332	rBV	1330983	1255220	29.81%	3.503%
14	10.322	1397	1400	1403	rVB	65319	48383	1.15%	0.135%
15	10.692	1455	1463	1466	rBV	2212869	2327131	55.26%	6.494%
16	10.792	1477	1480	1490	rBV	76897	80776	1.92%	0.225%
17	11.386	1577	1581	1585	rBV	1439602	1213086	28.81%	3.385%
18	11.598	1613	1617	1625	rBV2	85462	92761	2.20%	0.259%
19	12.422	1753	1757	1761	rBV	95054	95455	2.27%	0.266%
20	12.474	1761	1766	1769	rVB2	82649	71761	1.70%	0.200%
21	12.974	1846	1851	1854	rBV2	3349657	3714675	88.21%	10.367%
22	13.445	1926	1931	1934	rBV	486149	435226	10.34%	1.215%
23	13.857	1997	2001	2009	rBV	288637	323295	7.68%	0.902%
24	14.027	2026	2030	2033	rBV	1013312	902977	21.44%	2.520%
25	14.486	2103	2108	2115	rBV6	25391	46659	1.11%	0.130%
26	15.498	2274	2280	2289	rBV	565664	701438	16.66%	1.958%
27	17.545	2621	2628	2638	rBV8	17778	50455	1.20%	0.141%

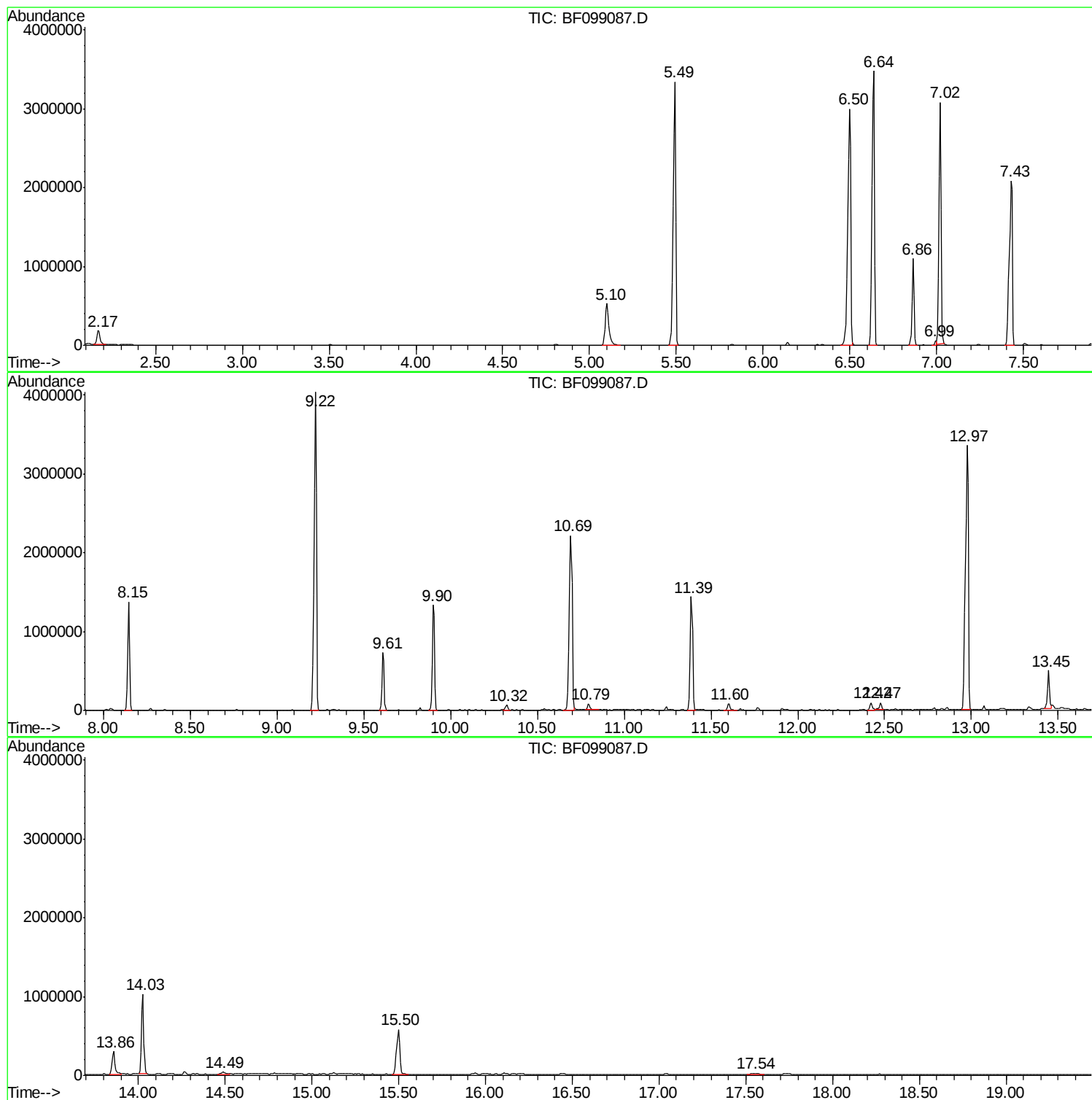
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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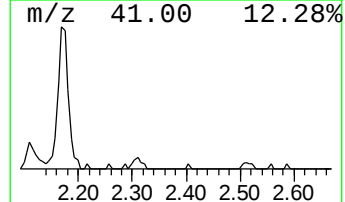
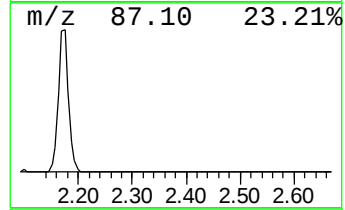
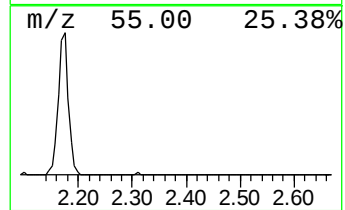
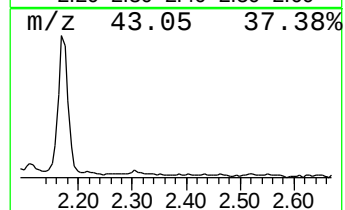
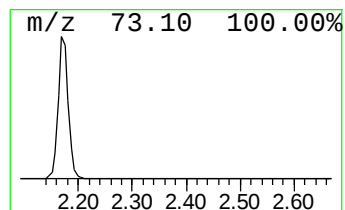
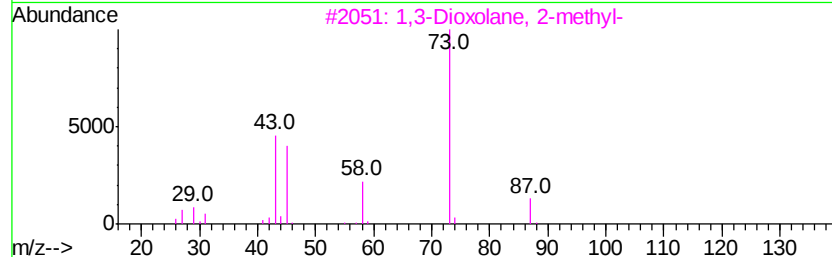
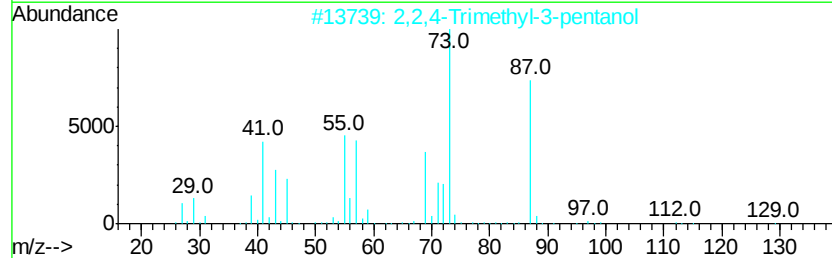
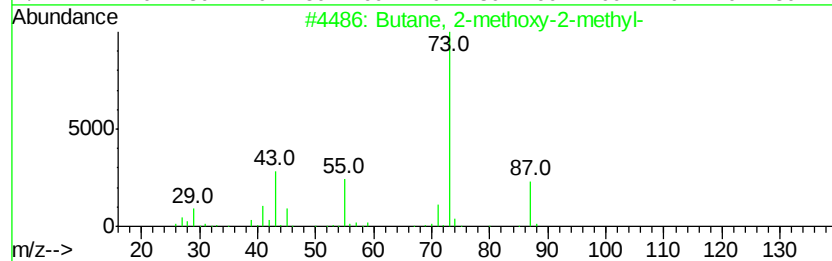
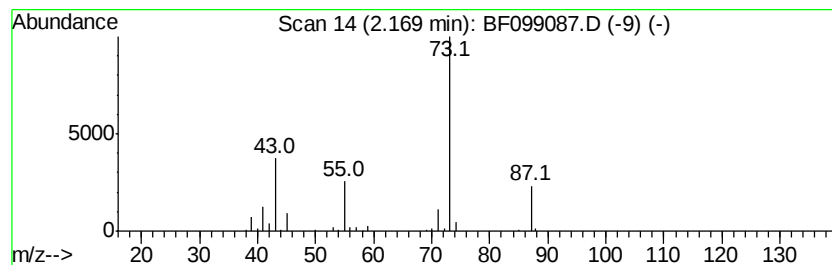
Instrument :
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ClientSampleId :
SASP2P-TP-106-T(0-5)

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.		
2.17	5.26 ng	236051	1,4-Dichlorobenzene-d4		6.86		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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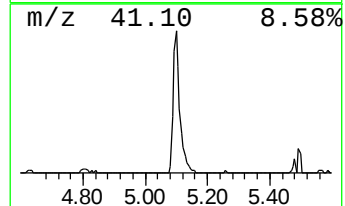
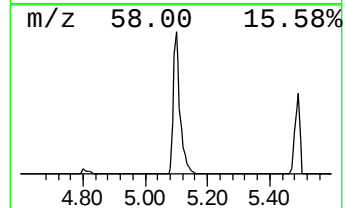
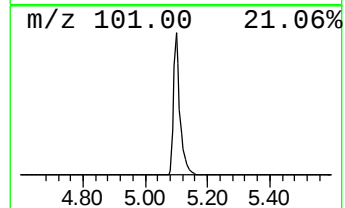
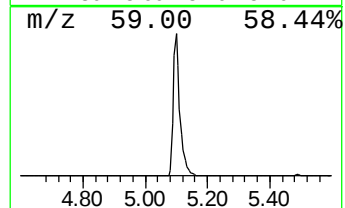
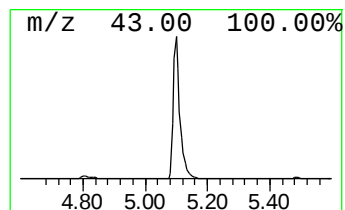
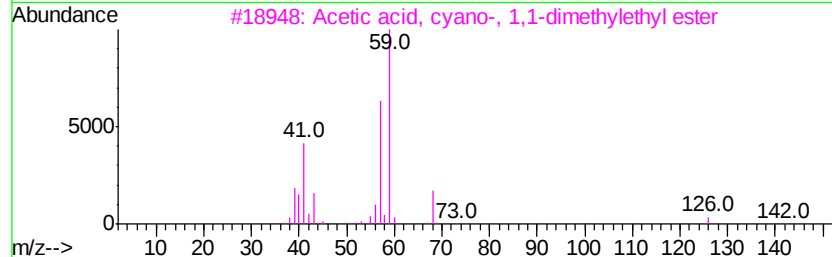
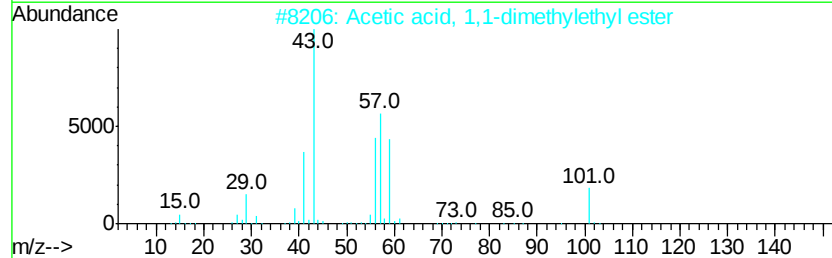
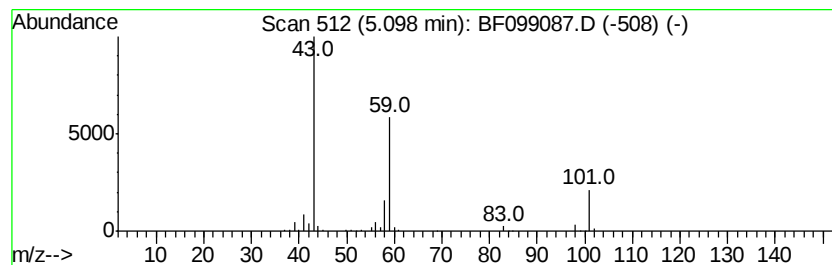
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	17.68 ng	792637	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	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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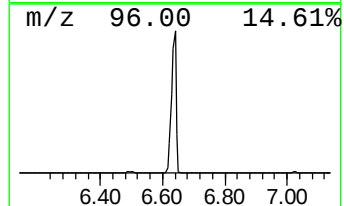
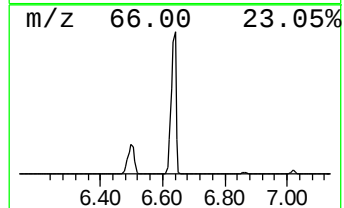
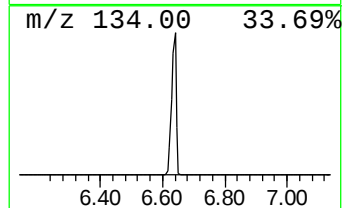
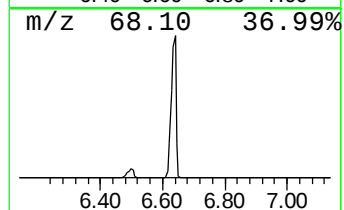
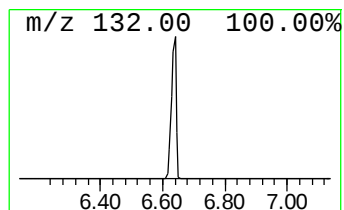
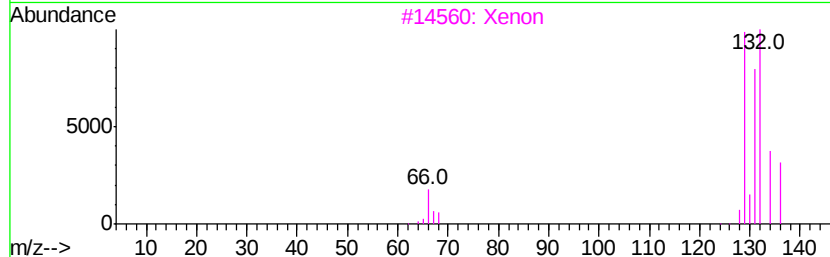
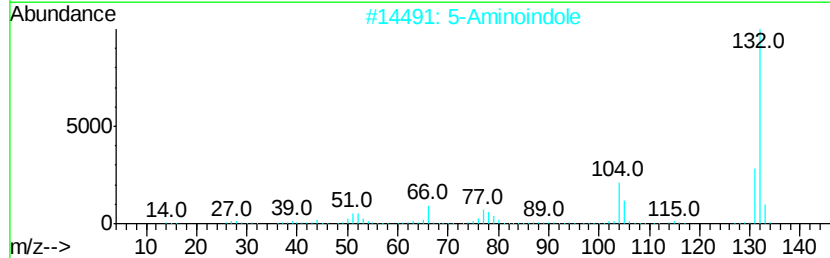
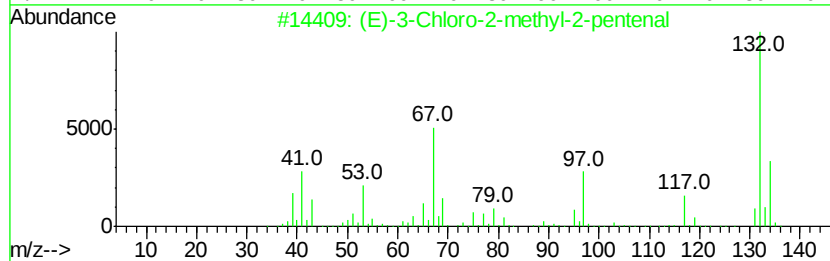
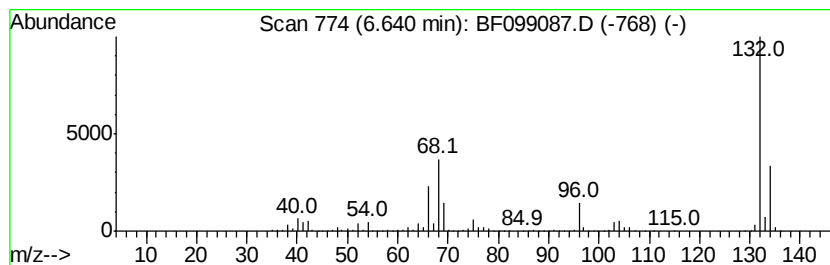
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Peak Number 3 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	83.21 ng	3731040	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Xenon	132	Xe	007440-63-3	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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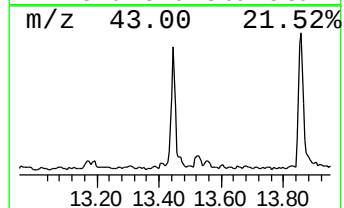
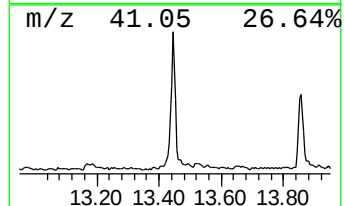
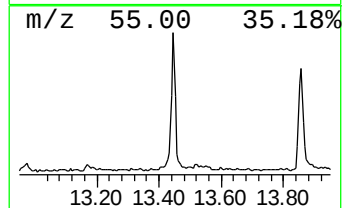
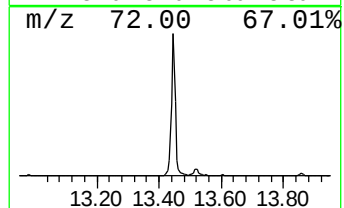
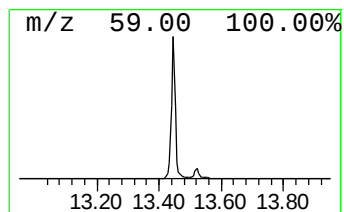
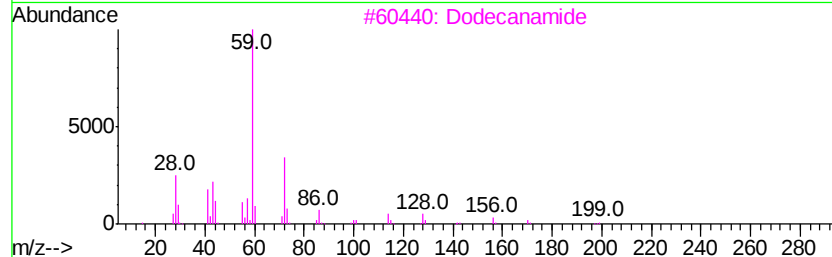
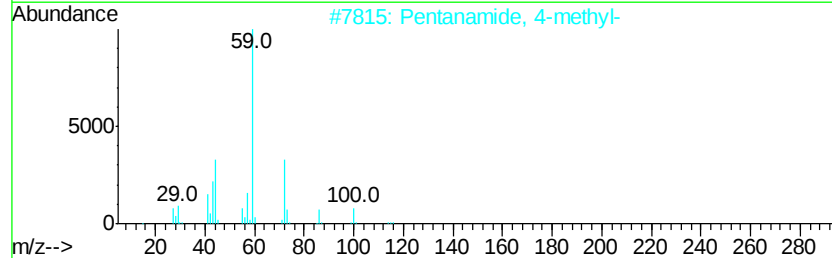
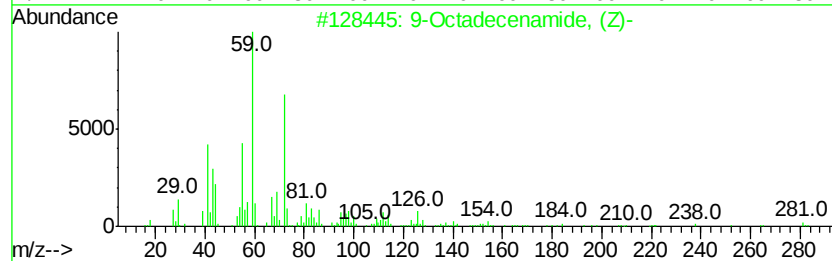
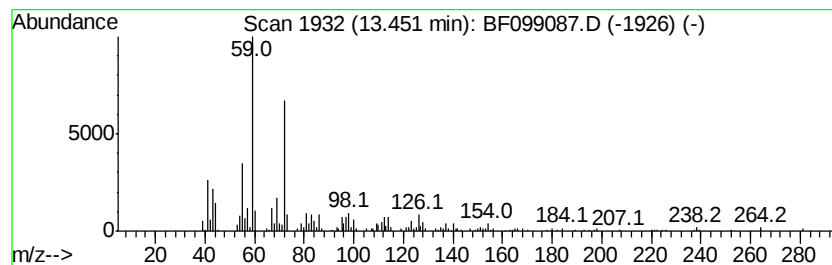
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	9.64 ng	435226	Chrysene-d12	14.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	59
3		Dodecanamide	199	C12H25NO	001120-16-7	59
4		Nonanamide	157	C9H19NO	001120-07-6	53
5		Octanamide	143	C8H17NO	000629-01-6	53



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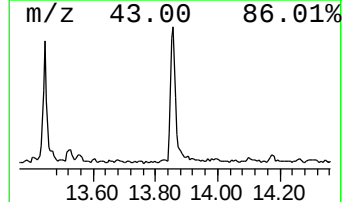
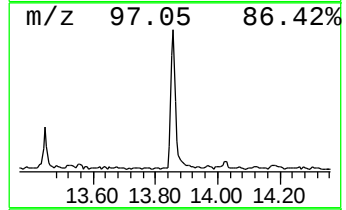
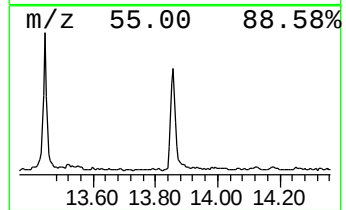
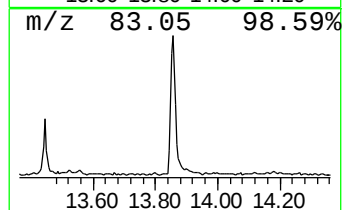
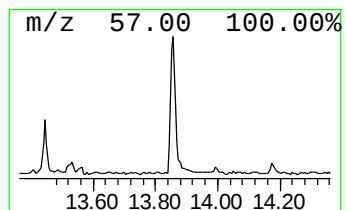
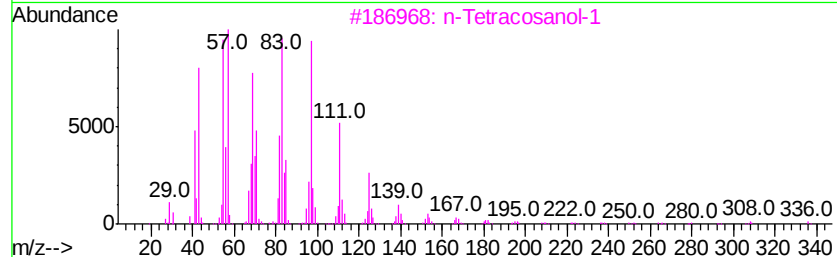
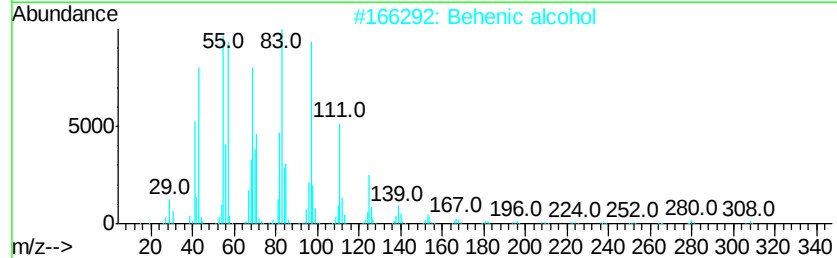
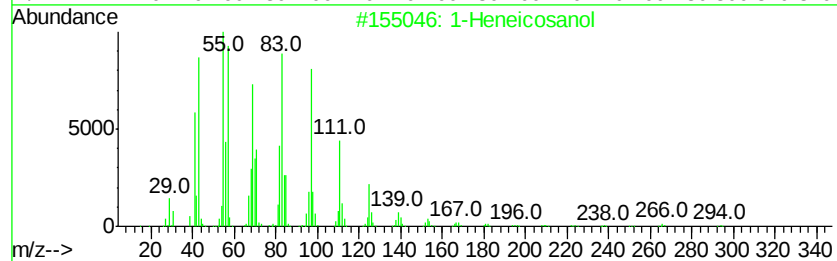
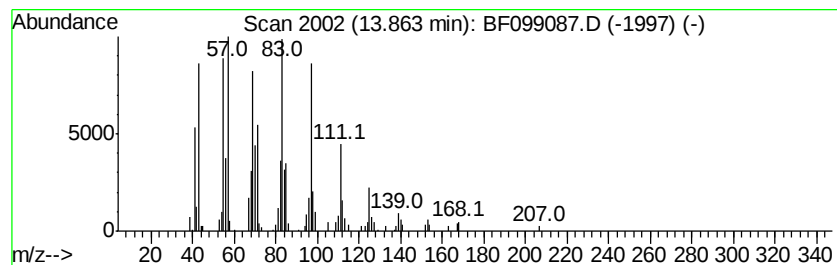
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Peak Number 6 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	7.16 ng	323295	Chrysene-d12	14.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Behenic alcohol	326	C22H46O	000661-19-8	95
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.17	5.3	ng	236051	1	6.86	896762	20.0
2-Pentanone, 4-hy...	5.10	17.7	ng	792637	1	6.86	896762	20.0
unknown6.64	6.64	83.2	ng	3731040	1	6.86	896762	20.0
9-Octadecenamide, ...	13.45	9.6	ng	435226	5	14.03	902977	20.0
1-Heneicosanol	13.86	7.2	ng	323295	5	14.03	902977	20.0