

Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
 Data File : BF096558.D
 Acq On : 7 Jul 2017 14:47
 Operator : SJ/MA
 Sample : I4064-06
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PET-BF003-01

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-BF070117.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	4.887	471	476	485	rBV	394708	538391	20.02%	2.274%
2	5.316	543	549	552	rBV	2491161	2646608	98.40%	11.180%
3	6.339	717	723	727	rBV	2543270	2683063	99.76%	11.334%
4	6.469	740	745	748	rBV	2720238	2588214	96.23%	10.933%
5	6.692	780	783	787	rBV	695451	637722	23.71%	2.694%
6	6.851	806	810	814	rBV	2028228	1923832	71.53%	8.127%
7	7.257	873	879	882	rBV	1711579	1659815	61.71%	7.011%
8	7.975	997	1001	1005	rBV	937623	877071	32.61%	3.705%
9	9.057	1179	1185	1188	rBV	2895534	2689579	100.00%	11.361%
10	9.445	1248	1251	1255	rBV	236853	185122	6.88%	0.782%
11	9.727	1294	1299	1303	rBV	1064617	935188	34.77%	3.950%
12	10.175	1372	1375	1378	rVB	45060	34027	1.27%	0.144%
13	10.516	1428	1433	1436	rBV	1613614	1555164	57.82%	6.569%
14	10.645	1452	1455	1463	rBV	50049	53882	2.00%	0.228%
15	11.204	1546	1550	1554	rBV	1004912	880900	32.75%	3.721%
16	12.792	1815	1820	1823	rBV2	2300866	2280549	84.79%	9.633%
17	13.692	1970	1973	1981	rBV	145941	157126	5.84%	0.664%
18	13.833	1993	1997	2001	rBV	703555	626684	23.30%	2.647%
19	14.592	2122	2126	2133	rBV	178408	179980	6.69%	0.760%
20	14.686	2139	2142	2145	rVB	31228	31380	1.17%	0.133%
21	15.233	2230	2235	2241	rBV	451914	509136	18.93%	2.151%

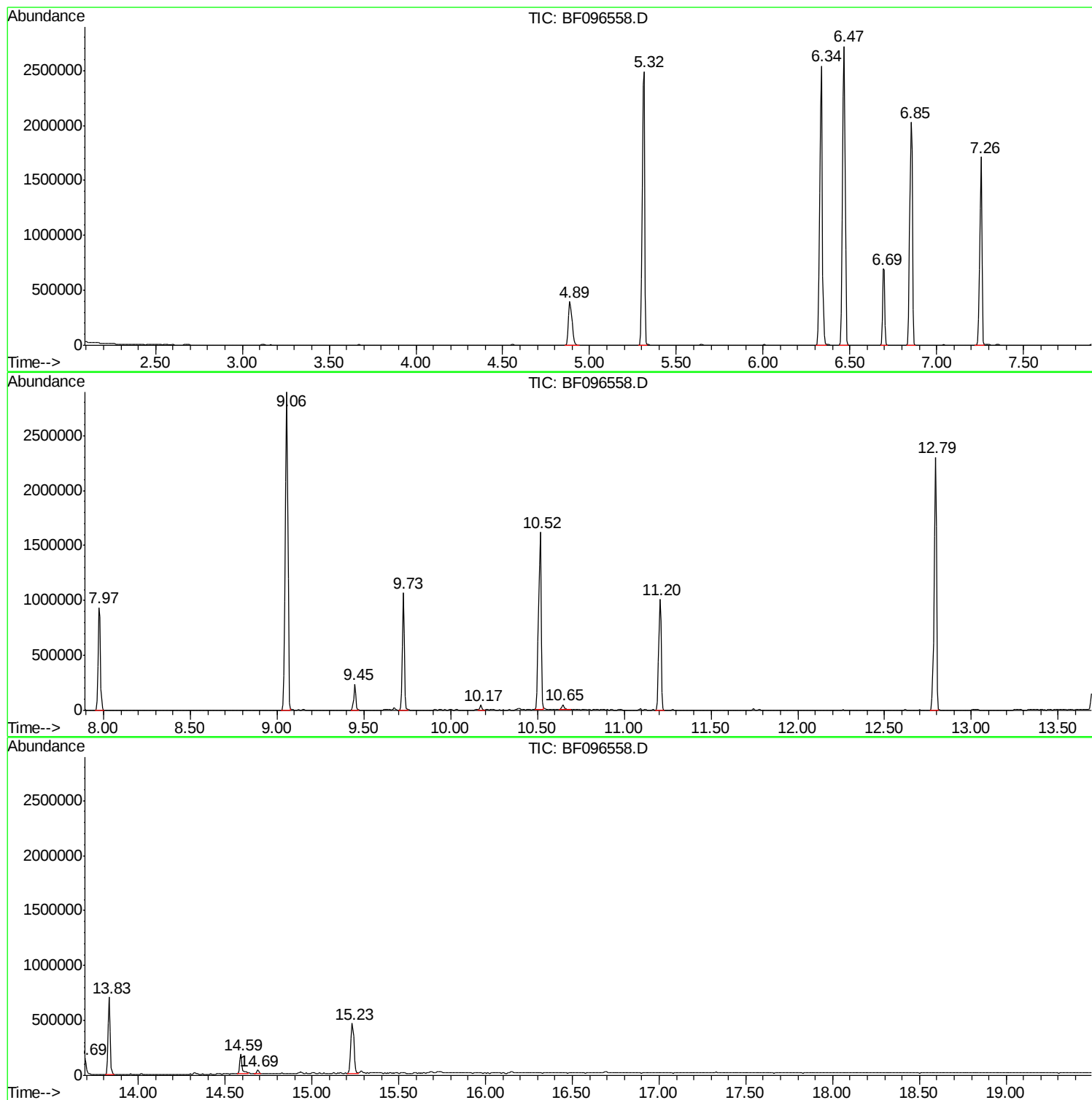
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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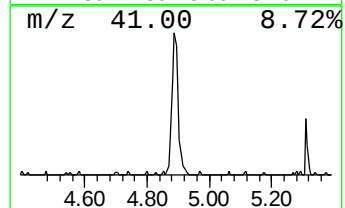
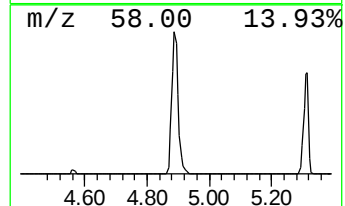
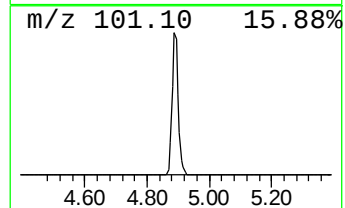
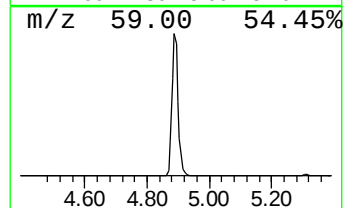
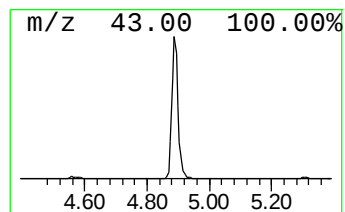
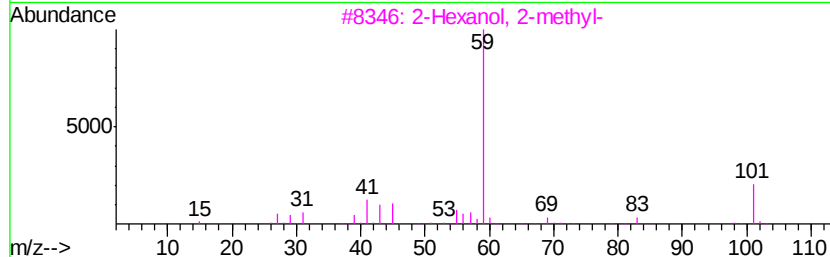
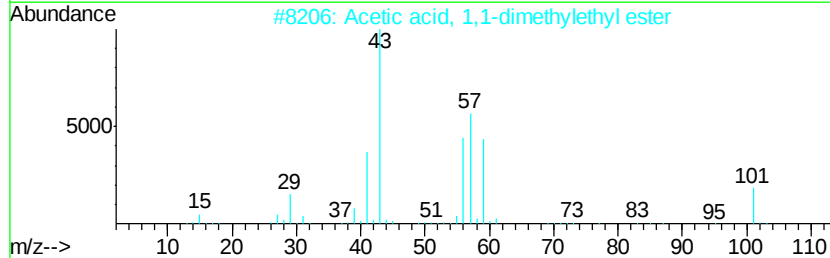
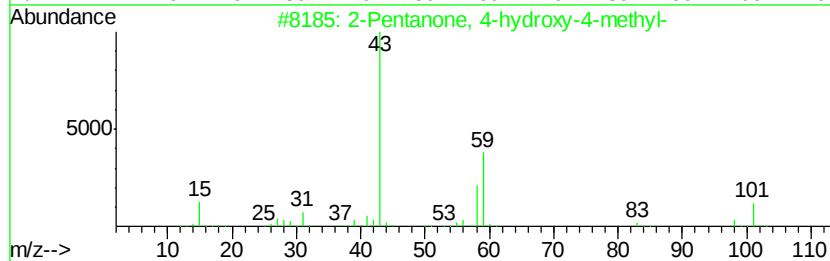
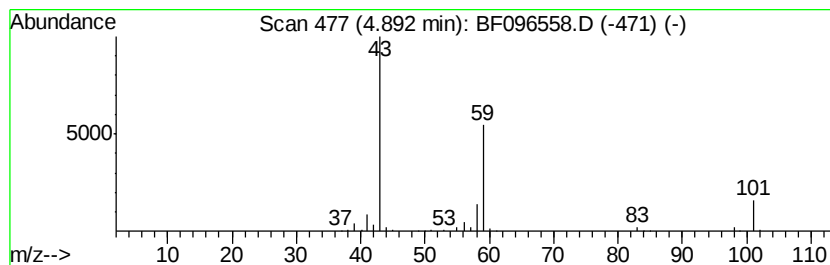
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	16.88 ng	538391	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			3-Hexanol	102	C6H14O	000623-37-0	33
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28



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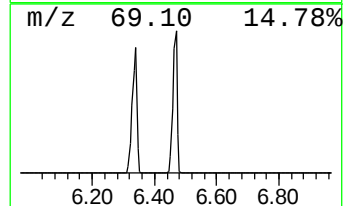
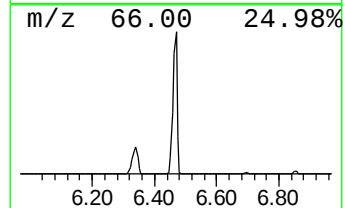
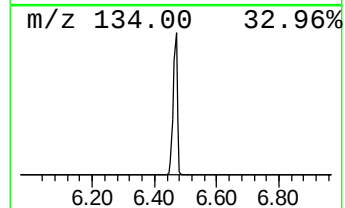
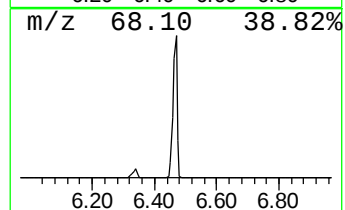
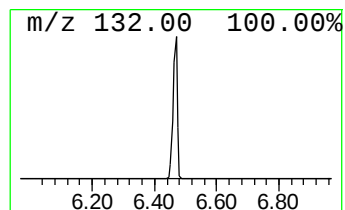
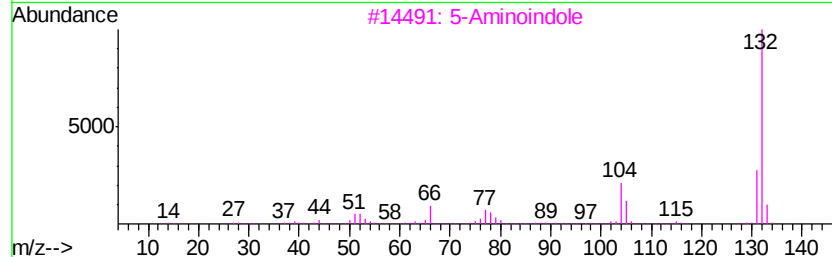
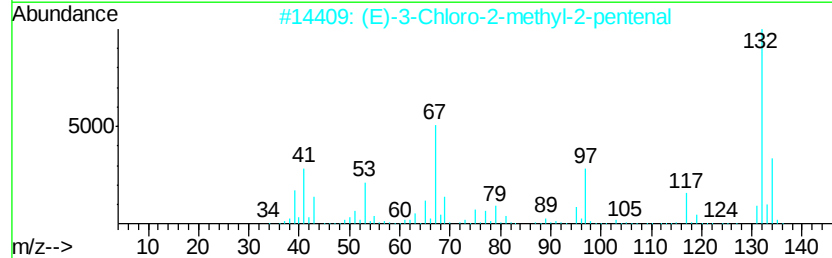
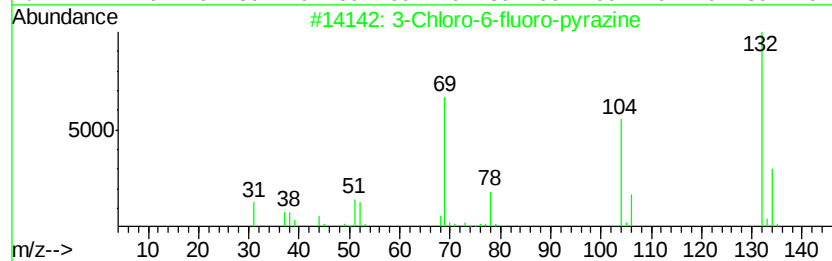
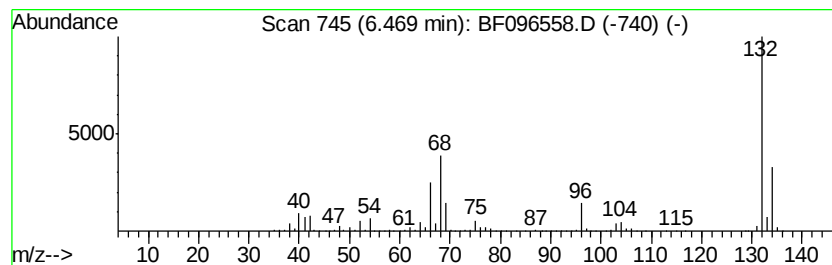
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Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	81.17 ng	2588210	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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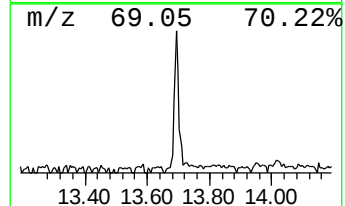
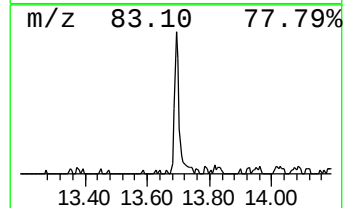
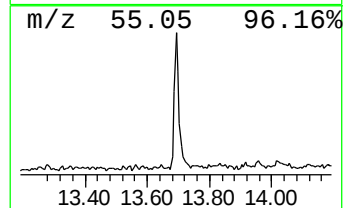
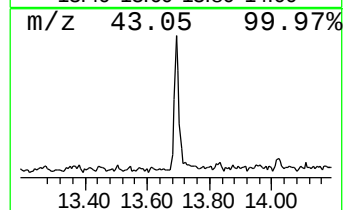
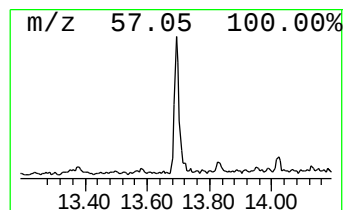
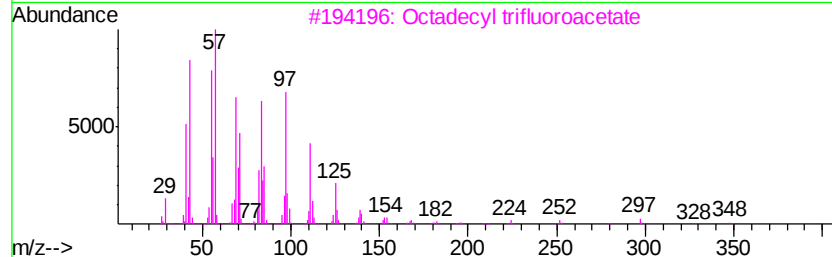
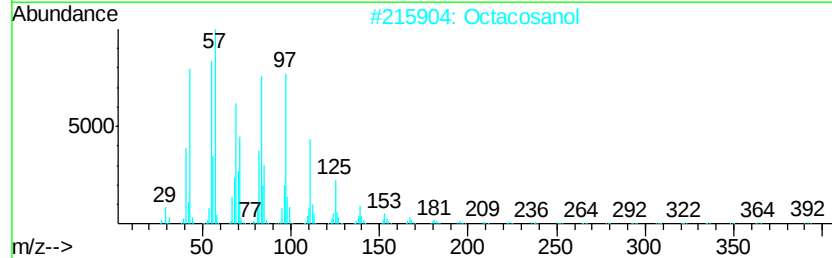
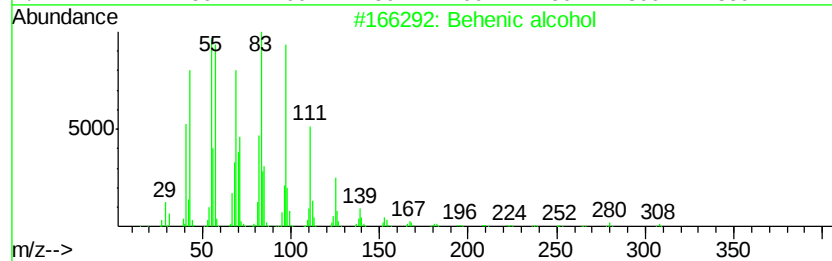
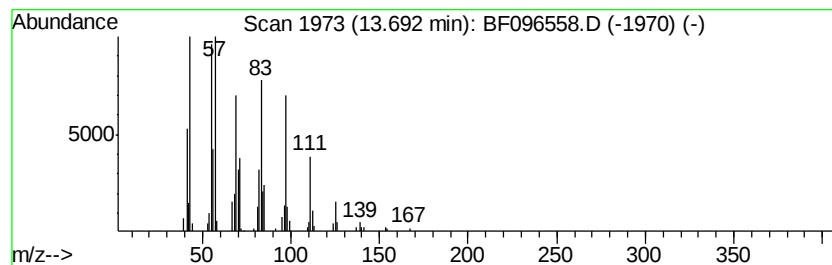
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Peak Number 4 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	5.01 ng	157126	Chrysene-d12	13.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	93
2		Octacosanol	410	C28H58O	000557-61-9	91
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4		1-Octadecanol	270	C18H38O	000112-92-5	91
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91



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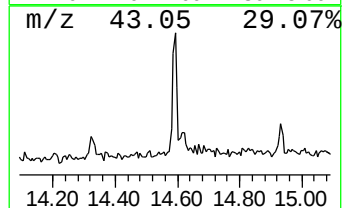
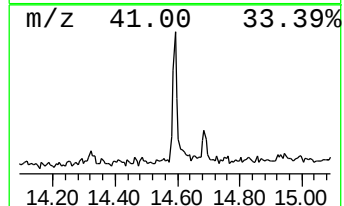
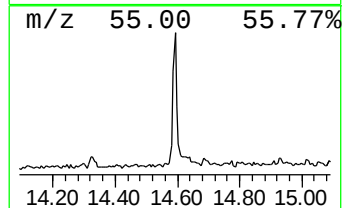
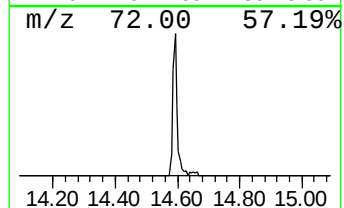
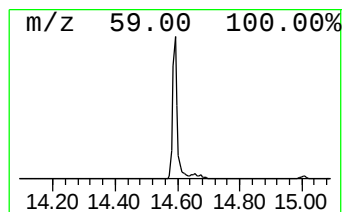
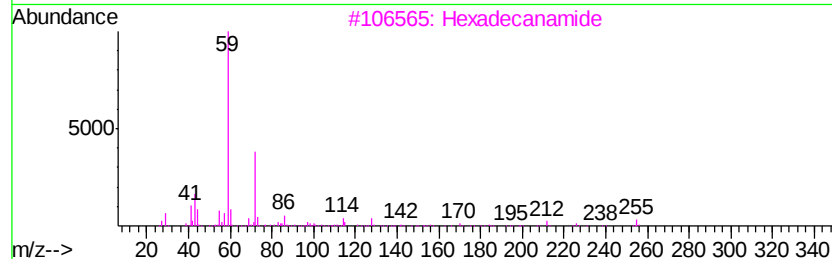
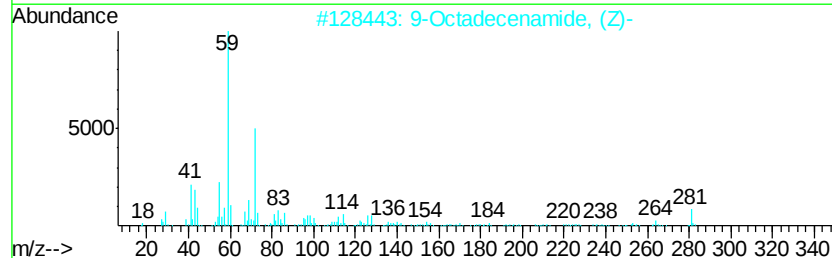
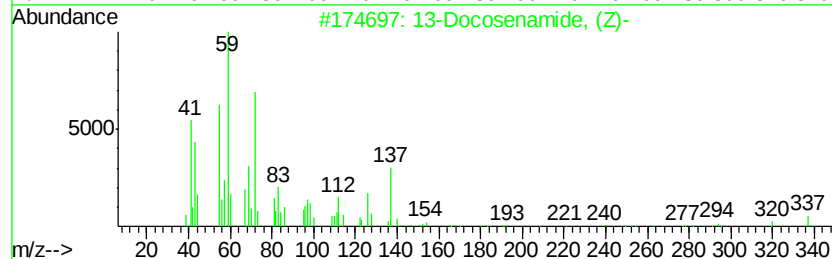
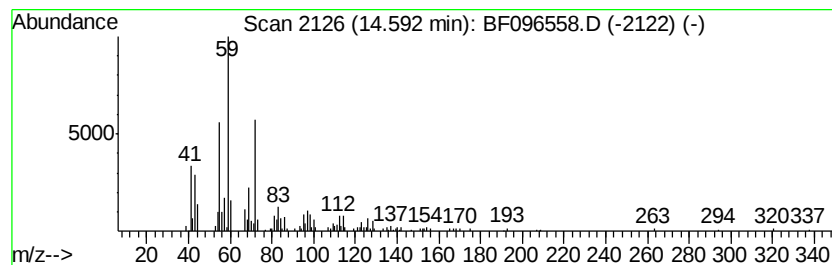
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Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	7.07 ng	179980	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3		Hexadecanamide	255	C16H33NO	000629-54-9	72
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	72
5		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	16.9	ng	538391	1	6.70	637722	20.0
unknown6.47	6.47	81.2	ng	2588210	1	6.70	637722	20.0
Behenic alcohol	13.69	5.0	ng	157126	5	13.83	626684	20.0
13-Docosenamide, ...	14.59	7.1	ng	179980	6	15.23	509136	20.0