

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041318\
 Data File : BF104509.D
 Acq On : 14 Apr 2018 7:04
 Operator : JU/SJ
 Sample : J2368-03
 Misc :
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 041118-JETB-E-D-S

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-BF040618.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	3.846	295	299	306	rVB	31023	39380	1.11%	0.195%
2	5.004	493	496	505	rVB	87350	87683	2.47%	0.434%
3	5.422	563	567	570	rBV	1140733	959547	26.98%	4.745%
4	6.028	668	670	681	rBV	56868	62792	1.77%	0.311%
5	6.440	736	740	747	rBV	698009	607690	17.09%	3.005%
6	6.575	759	763	767	rBV	1945841	1788705	50.30%	8.846%
7	6.810	799	803	806	rBV	819987	703888	19.79%	3.481%
8	6.963	825	829	833	rBV	2605291	2520320	70.87%	12.464%
9	7.375	893	899	902	rBV	1968933	2017710	56.74%	9.979%
10	8.092	1017	1021	1024	rBV	1126840	924705	26.00%	4.573%
11	9.169	1199	1204	1207	rBV	3656767	3556227	100.00%	17.587%
12	9.557	1267	1270	1274	rBV	73363	65987	1.86%	0.326%
13	9.845	1314	1319	1328	rBV2	1062596	969635	27.27%	4.795%
14	10.275	1388	1392	1395	rVB	45825	36783	1.03%	0.182%
15	10.639	1450	1454	1465	rVB	1257294	1162192	32.68%	5.748%
16	11.333	1568	1572	1576	rBV	867683	767718	21.59%	3.797%
17	12.739	1808	1811	1815	rBV	108341	89894	2.53%	0.445%
18	12.927	1838	1843	1846	rBV	2699246	2581846	72.60%	12.768%
19	13.451	1928	1932	1935	rBV	64760	56969	1.60%	0.282%
20	13.821	1991	1995	2002	rBV	79087	90827	2.55%	0.449%
21	13.980	2018	2022	2026	rBV	749722	638704	17.96%	3.159%
22	15.451	2266	2272	2280	rBV	355639	491308	13.82%	2.430%

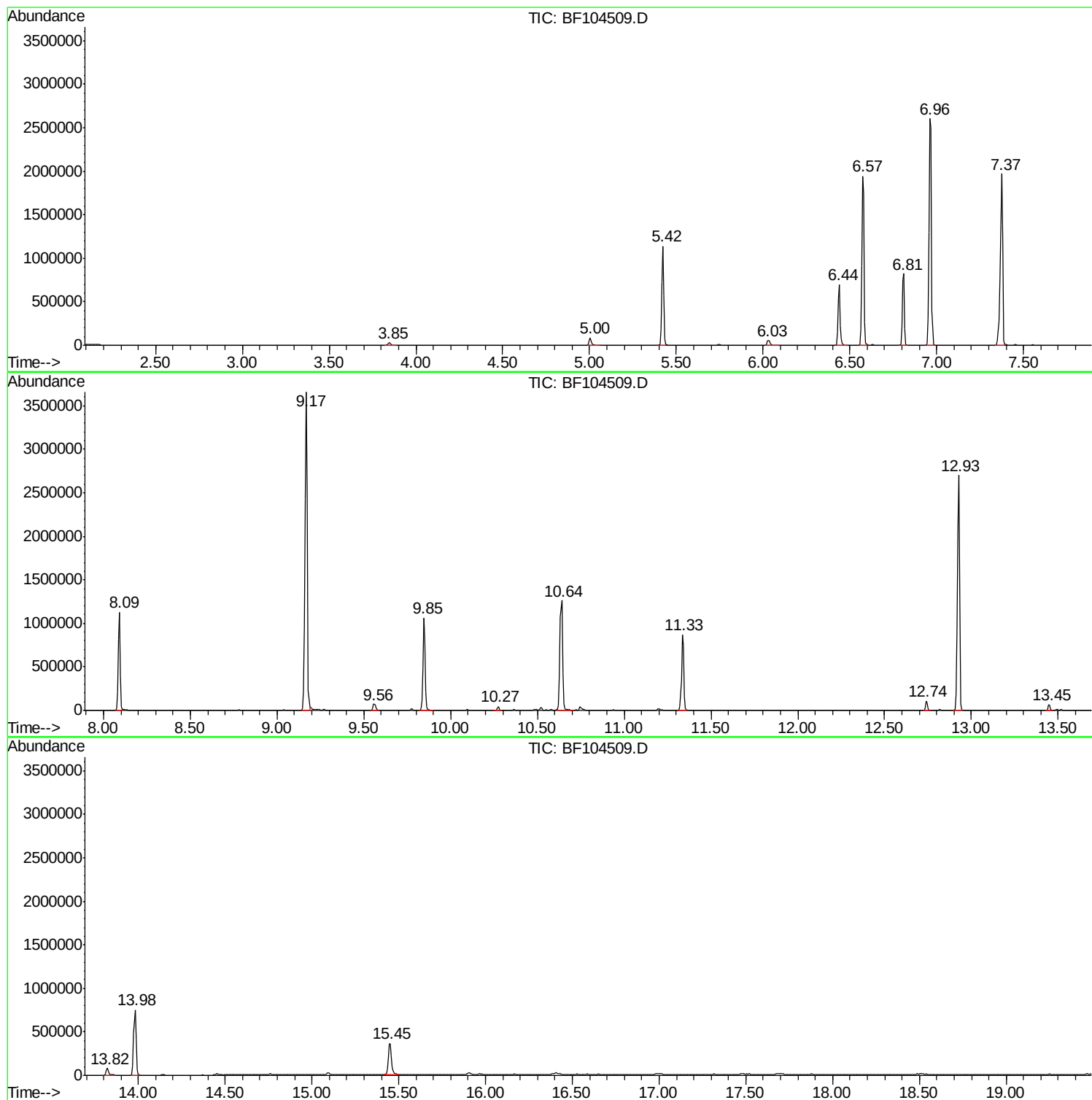
Sum of corrected areas: 20220510

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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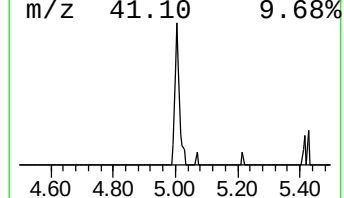
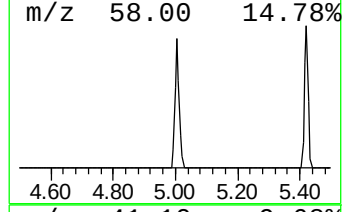
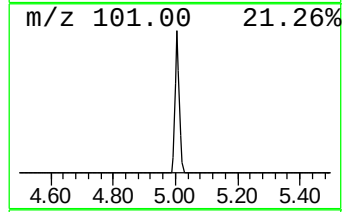
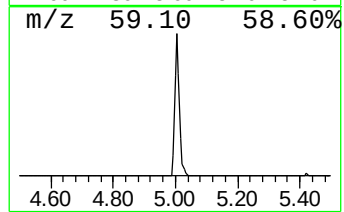
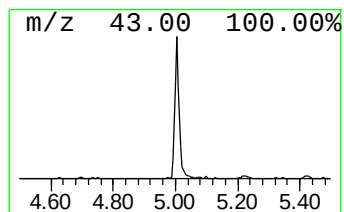
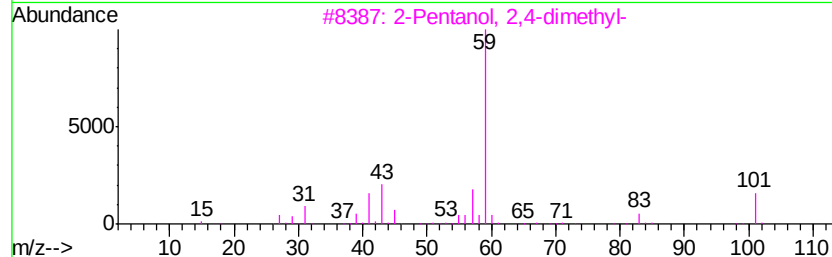
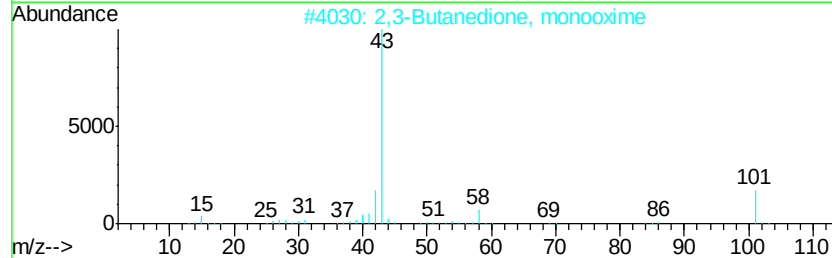
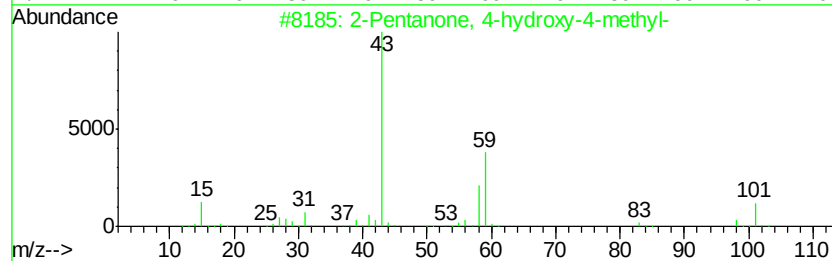
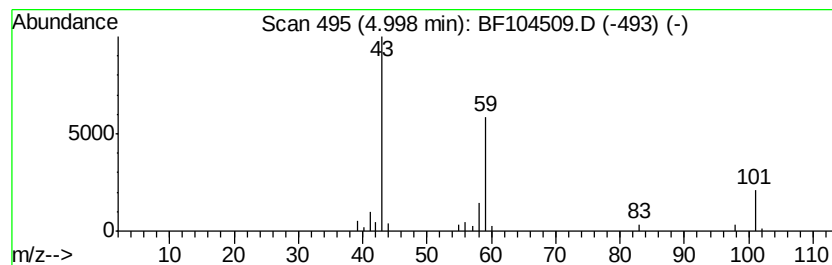
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	2.49 ng	87683	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	28
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
5	1,2-Butanediol	90	C4H10O2	000584-03-2	23



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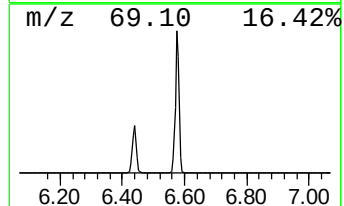
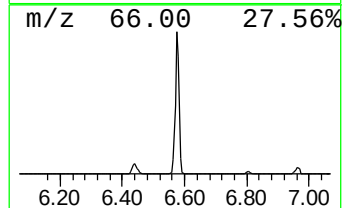
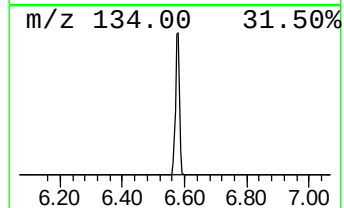
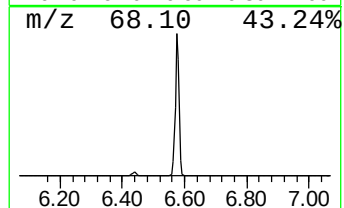
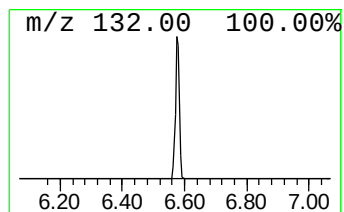
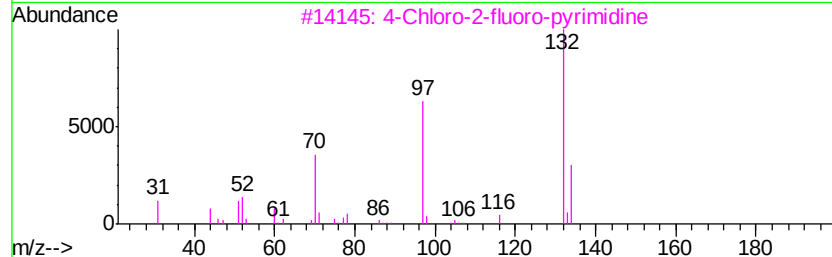
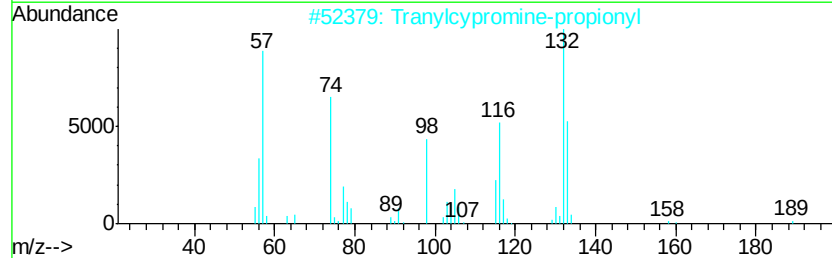
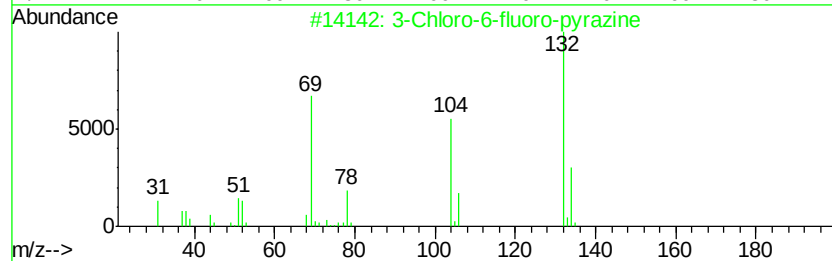
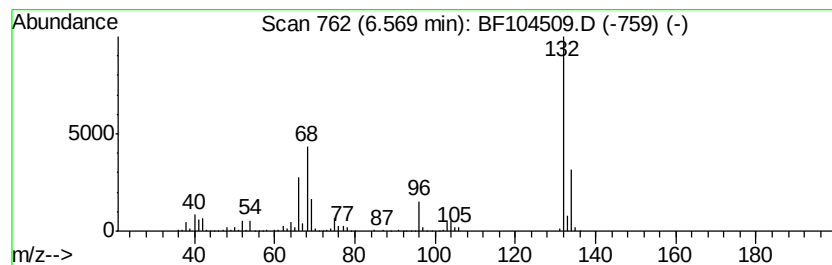
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Peak Number 2 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	50.82 ng	1788710	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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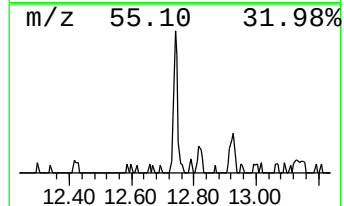
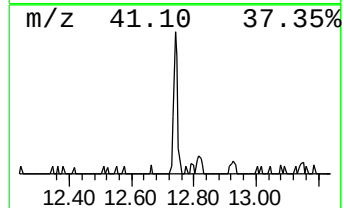
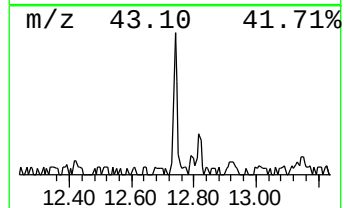
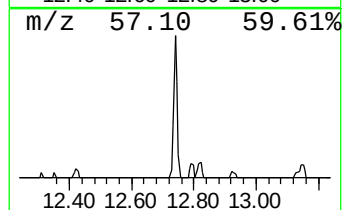
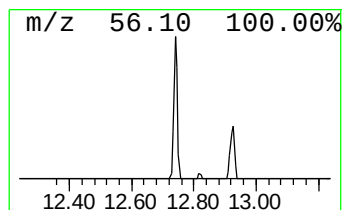
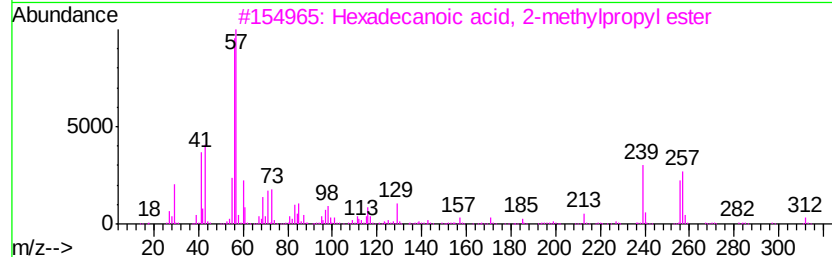
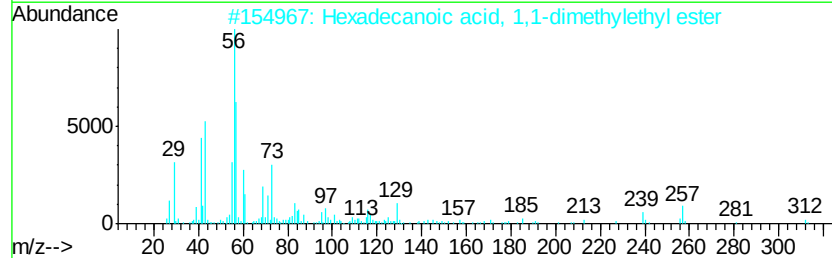
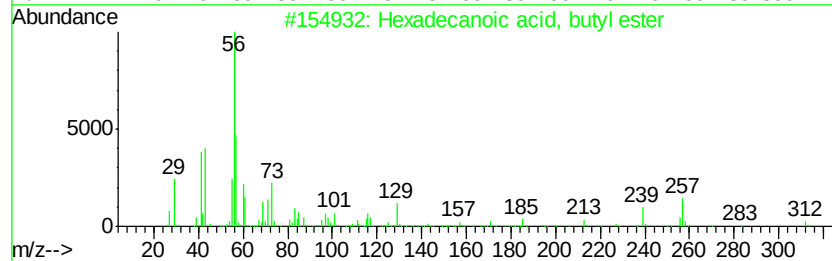
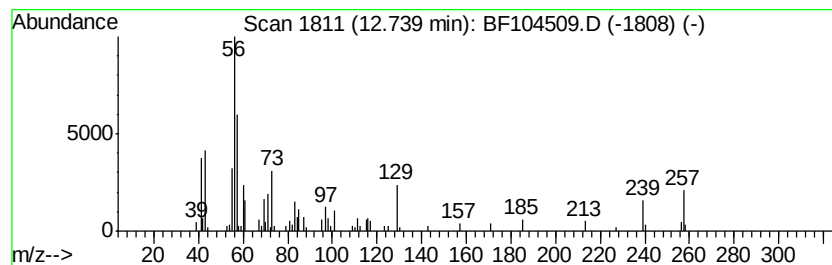
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	2.81 ng	89894	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	40
4		Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35
5		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	27



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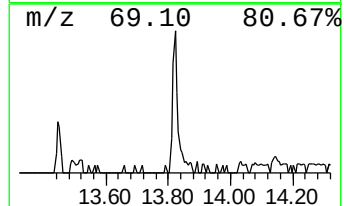
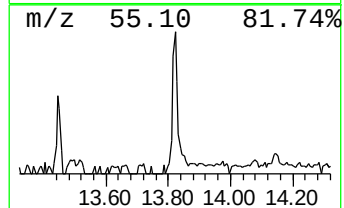
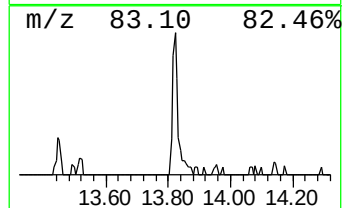
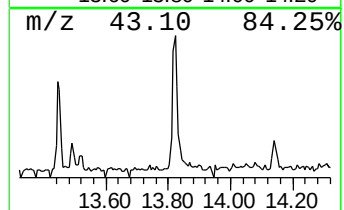
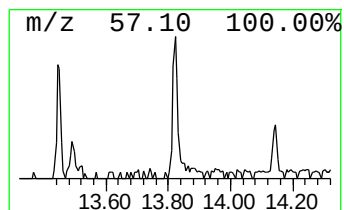
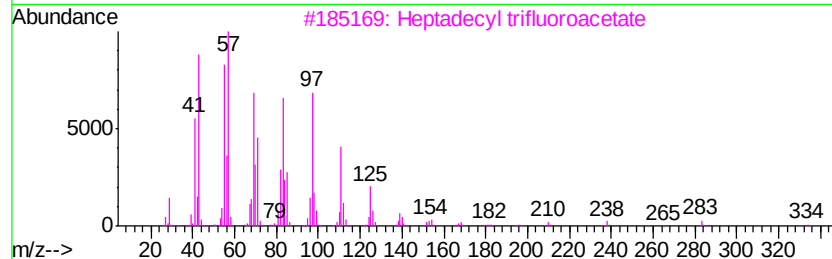
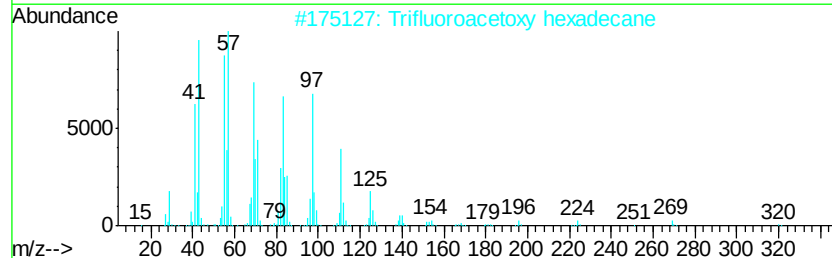
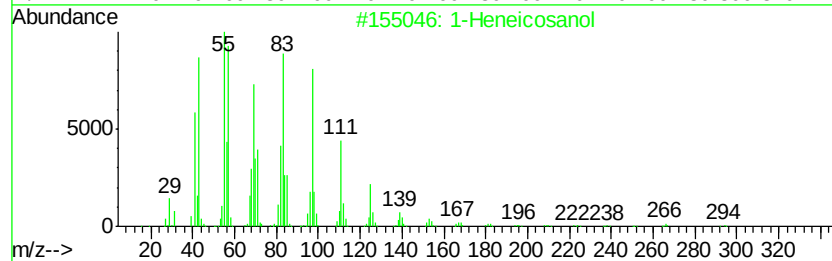
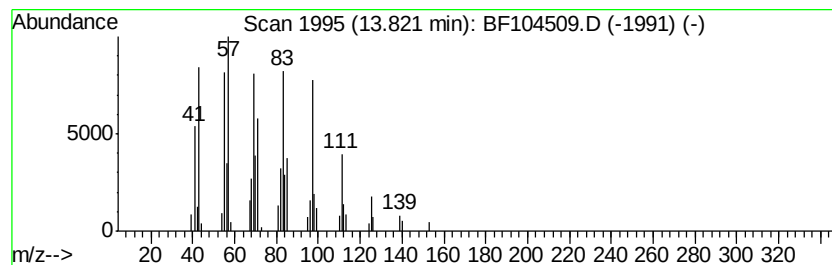
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Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.82	2.84 ng	90827	Chrysene-d12	13.98	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	2.5	ng	87683	1	6.81	703888	20.0
unknown6.57	6.57	50.8	ng	1788710	1	6.81	703888	20.0
Hexadecanoic acid...	12.74	2.8	ng	89894	5	13.98	638704	20.0
1-Heneicosanol	13.82	2.8	ng	90827	5	13.98	638704	20.0