

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122117\
 Data File : BF101645.D
 Acq On : 22 Dec 2017 9:49
 Operator : SJ/JU
 Sample : I7008-11
 Misc :
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 121817-TIFR-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-BF121417.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	5.010	494	497	513	rBV	74302	128627	3.81%	0.586%
2	5.416	563	566	587	rBV	742913	1240173	36.73%	5.648%
3	6.440	737	740	758	rBV2	520226	937428	27.76%	4.269%
4	6.569	758	762	769	rBV	2131313	2105374	62.35%	9.589%
5	6.798	797	801	809	rBV	828767	823620	24.39%	3.751%
6	6.951	823	827	842	rBV	2883642	2802957	83.01%	12.766%
7	7.369	894	898	922	rBV	2048801	2335507	69.17%	10.637%
8	8.081	1015	1019	1037	rBV	868843	988452	29.27%	4.502%
9	9.151	1197	1201	1204	rBV	3673348	3376468	100.00%	15.378%
10	9.834	1314	1317	1337	rVB	895681	870980	25.80%	3.967%
11	10.628	1448	1452	1465	rBV	1087450	1129480	33.45%	5.144%
12	11.322	1567	1570	1580	rBV	703421	741509	21.96%	3.377%
13	12.710	1803	1806	1809	rBV	155793	123852	3.67%	0.564%
14	12.904	1835	1839	1842	rBV	2860368	2602404	77.07%	11.852%
15	13.416	1922	1926	1929	rBV	103698	97792	2.90%	0.445%
16	13.792	1986	1990	1998	rBV2	31508	57074	1.69%	0.260%
17	13.969	2017	2020	2028	rBV	833898	898487	26.61%	4.092%
18	14.404	2091	2094	2098	rBV	35272	36753	1.09%	0.167%
19	15.439	2265	2270	2282	rVB	473187	660039	19.55%	3.006%

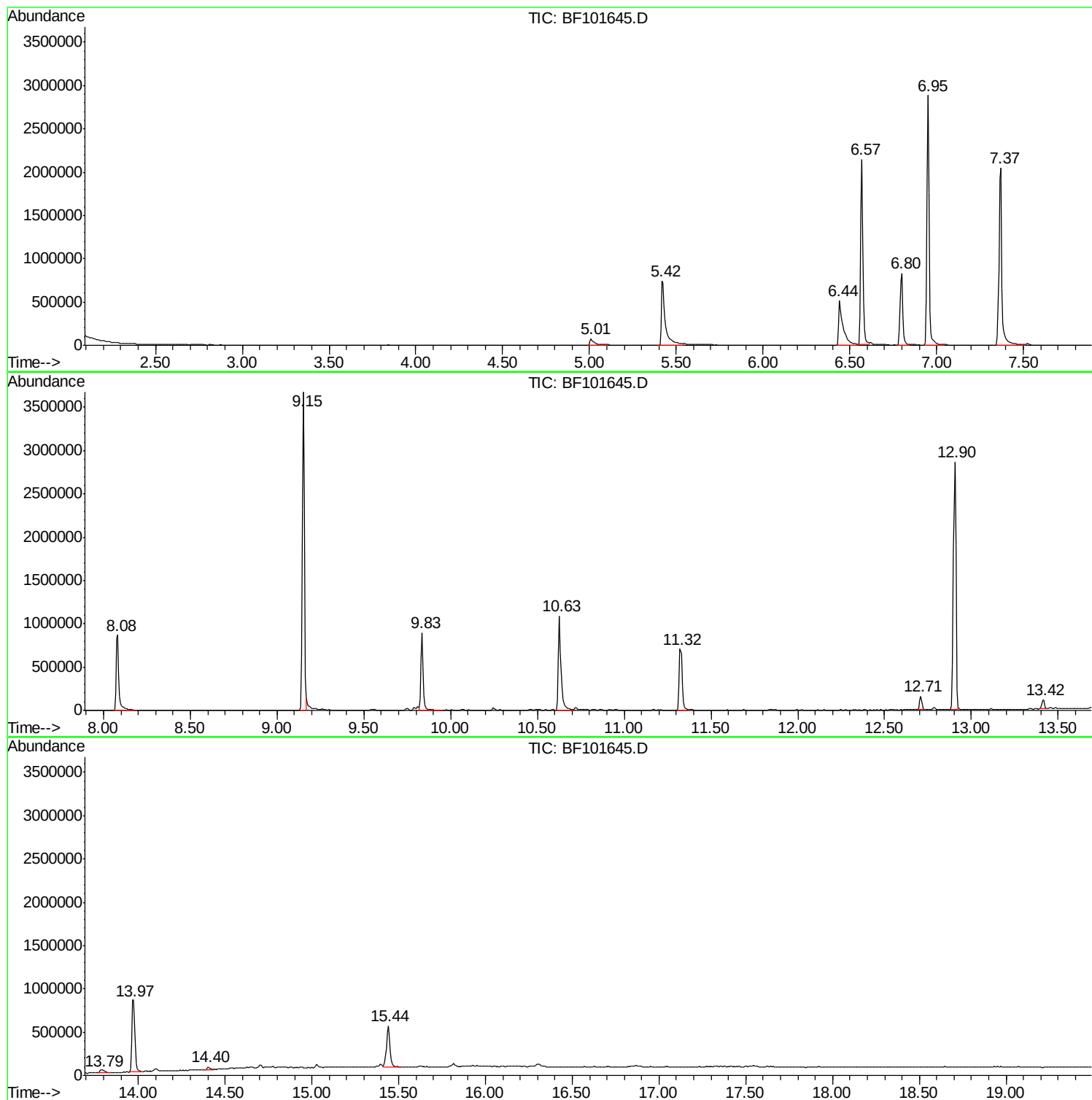
Sum of corrected areas: 21956976

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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121417.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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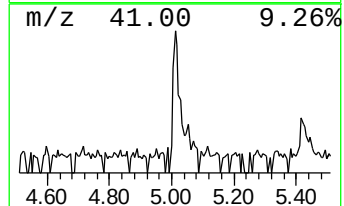
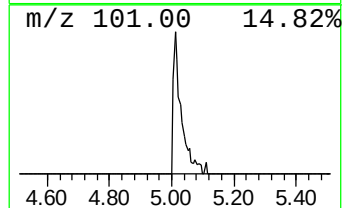
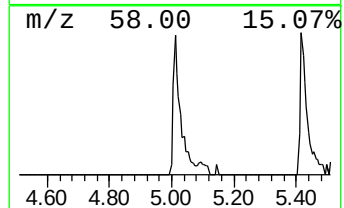
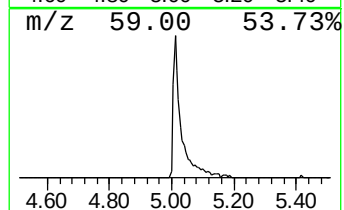
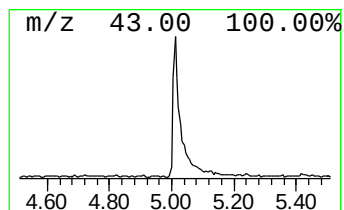
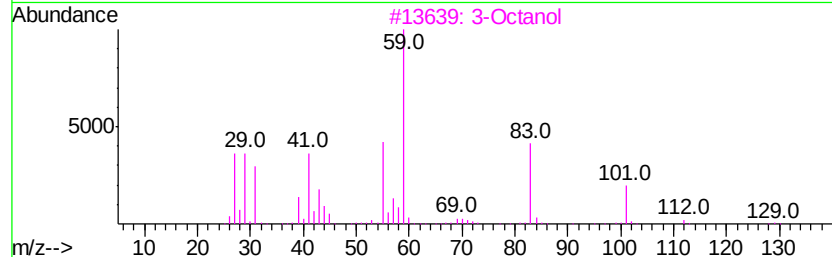
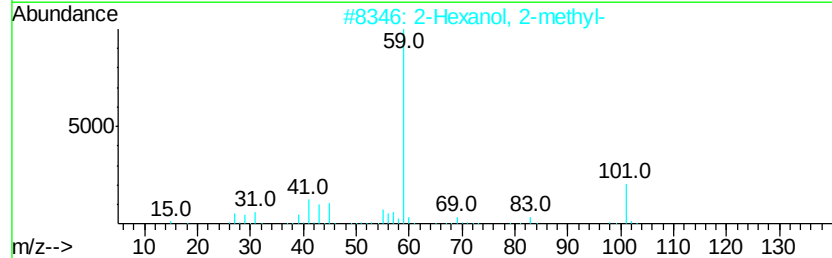
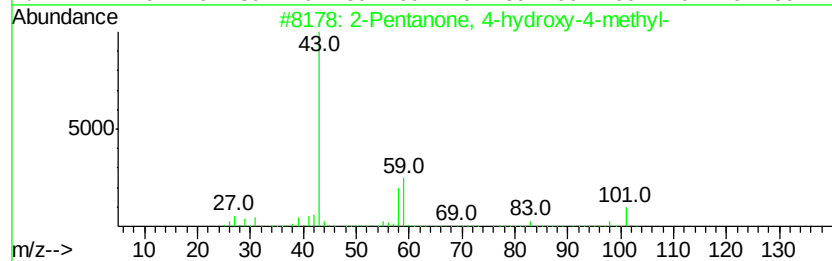
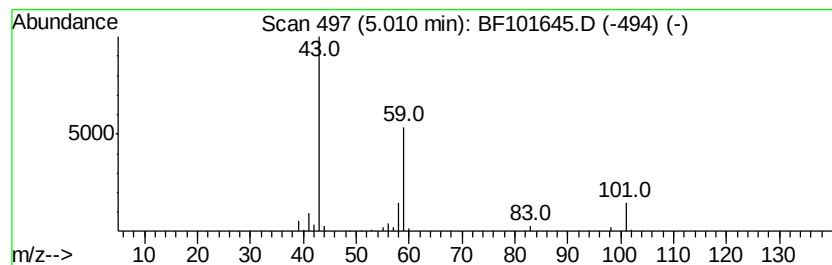
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
5.01	3.12 ng	128627	1,4-Dichlorobenzene-d4	6.80	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3	3-Octanol	130	C8H18O	000589-98-0	33
4	3-Hexanol	102	C6H14O	000623-37-0	33
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25



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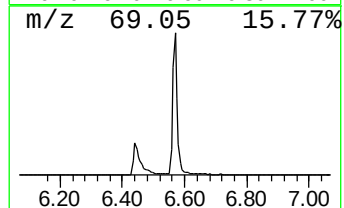
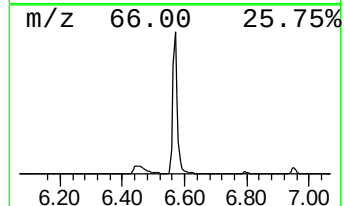
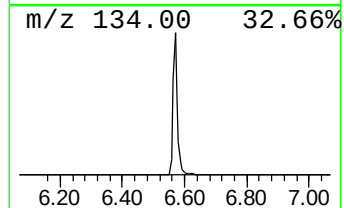
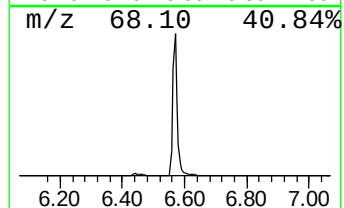
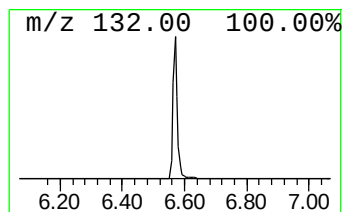
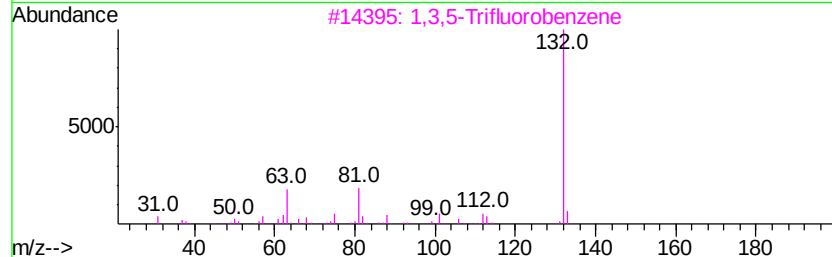
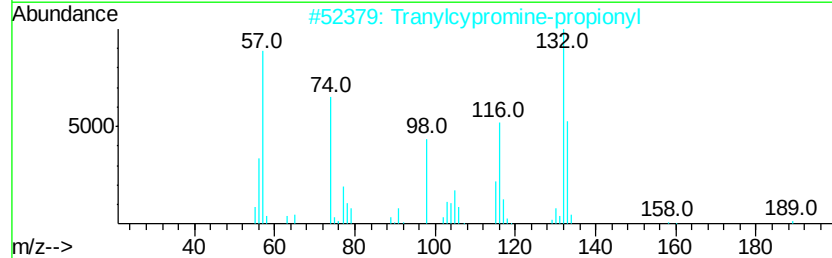
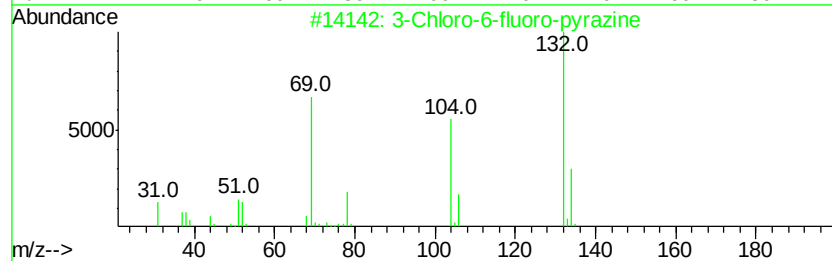
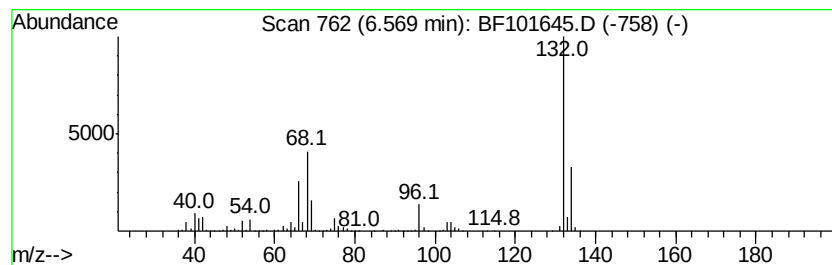
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Peak Number 2 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	51.12 ng	2105370	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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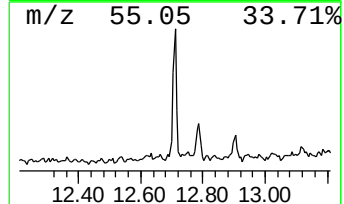
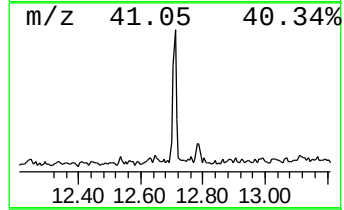
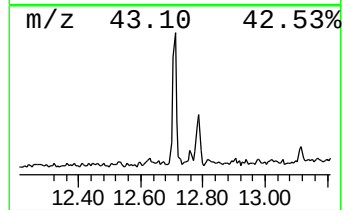
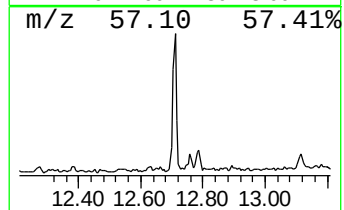
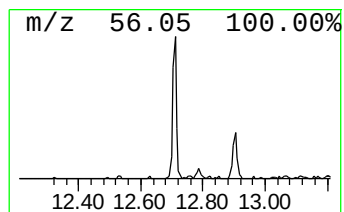
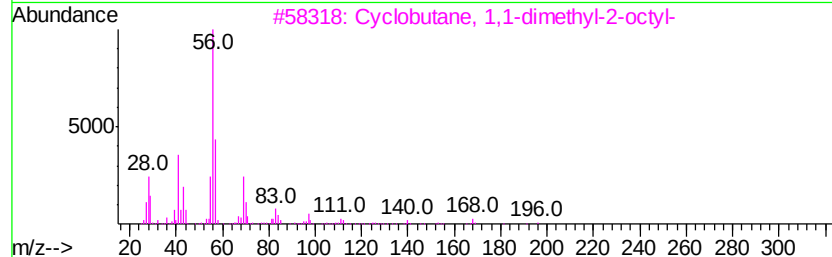
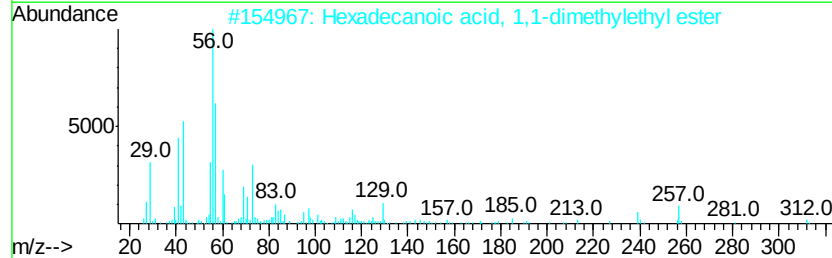
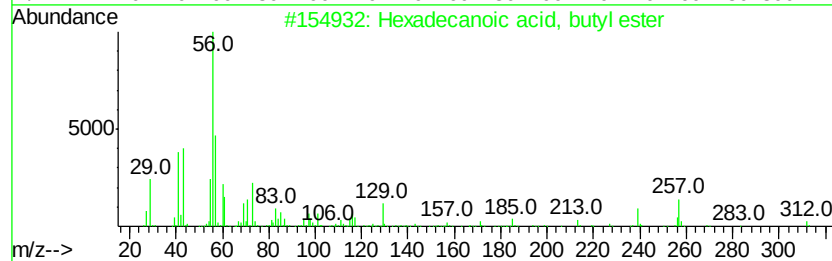
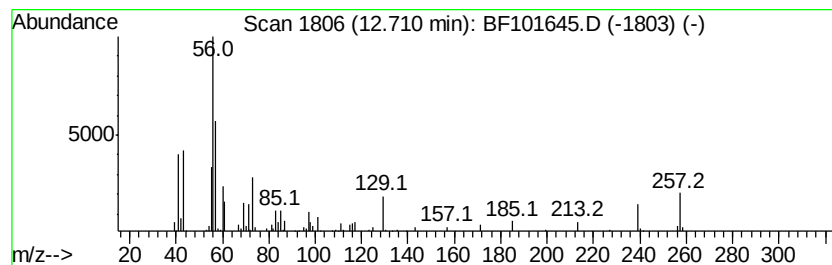
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	2.76 ng	123852	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	87
3		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
4		1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	37
5		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35



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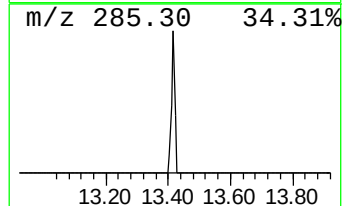
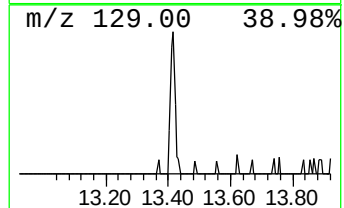
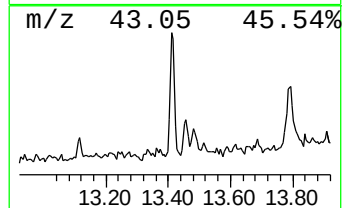
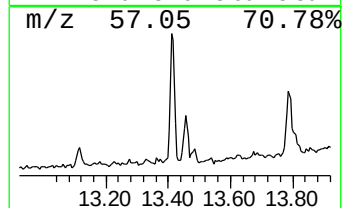
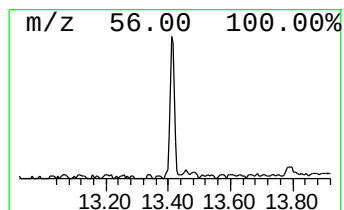
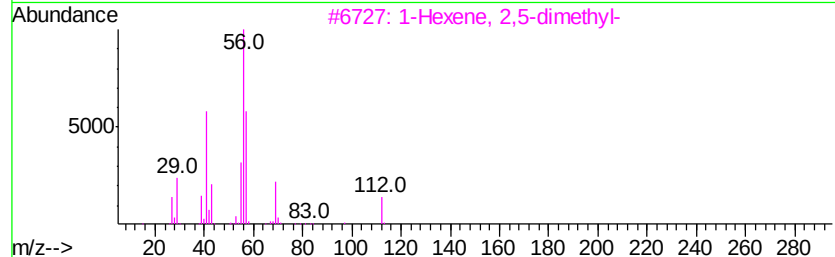
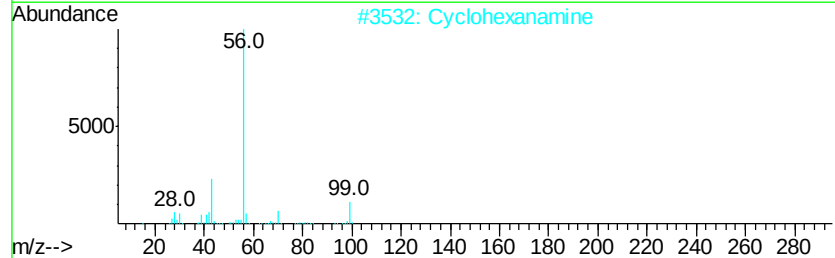
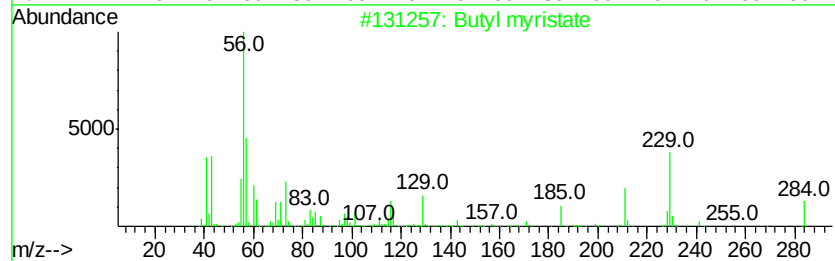
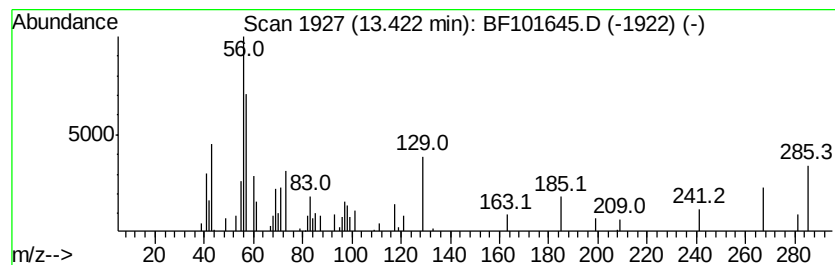
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Peak Number 5 Butyl myristate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.42	2.18 ng	97792	Chrysene-d12		13.97
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	74
2	Cyclohexanamine	99	C6H13N	000108-91-8	30
3	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27
4	4-t-Butylcyclohexylamine	155	C10H21N	005400-88-4	27
5	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.01	3.1	ng	128627	1	6.80	823620	20.0
unknown6.57	6.57	51.1	ng	2105370	1	6.80	823620	20.0
Hexadecanoic acid...	12.71	2.8	ng	123852	5	13.97	898487	20.0
Butyl myristate	13.42	2.2	ng	97792	5	13.97	898487	20.0