

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
 Data File : BF093651.D
 Acq On : 14 Mar 2017 11:45
 Operator : SJ/MA
 Sample : PB97542BL
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB97542BL

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-BF030717.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	4.859	258	260	284	rBV	686178	1503609	28.35%	3.387%
2	5.304	297	299	327	rBV	3577422	5303343	100.00%	11.945%
3	5.716	333	335	342	rVB	28023	59467	1.12%	0.134%
4	6.367	390	392	400	rBV	4095284	4839869	91.26%	10.901%
5	6.482	400	402	405	rVB	4355497	4630295	87.31%	10.429%
6	6.710	420	422	430	rVB	1041236	1134506	21.39%	2.555%
7	6.859	433	435	450	rVB	3512327	3673758	69.27%	8.274%
8	7.282	470	472	495	rBV	2546895	3239342	61.08%	7.296%
9	8.002	533	535	549	rVB	1477921	1531711	28.88%	3.450%
10	9.076	627	629	632	rBV	3494855	5118726	96.52%	11.529%
11	9.762	686	689	696	rBV	1409882	1688443	31.84%	3.803%
12	10.551	756	758	771	rBV2	2125341	2737005	51.61%	6.165%
13	11.248	817	819	830	rBV	1674176	1644574	31.01%	3.704%
14	12.654	940	942	945	rBV	219071	190414	3.59%	0.429%
15	12.836	955	958	961	rBV	4253261	4362005	82.25%	9.825%
16	13.362	1002	1004	1006	rBV	127892	140435	2.65%	0.316%
17	13.888	1048	1050	1059	rBV	1032137	1461033	27.55%	3.291%
18	15.294	1171	1173	1182	rVB	686419	1066461	20.11%	2.402%
19	15.500	1185	1191	1197	rBV3	18761	73650	1.39%	0.166%

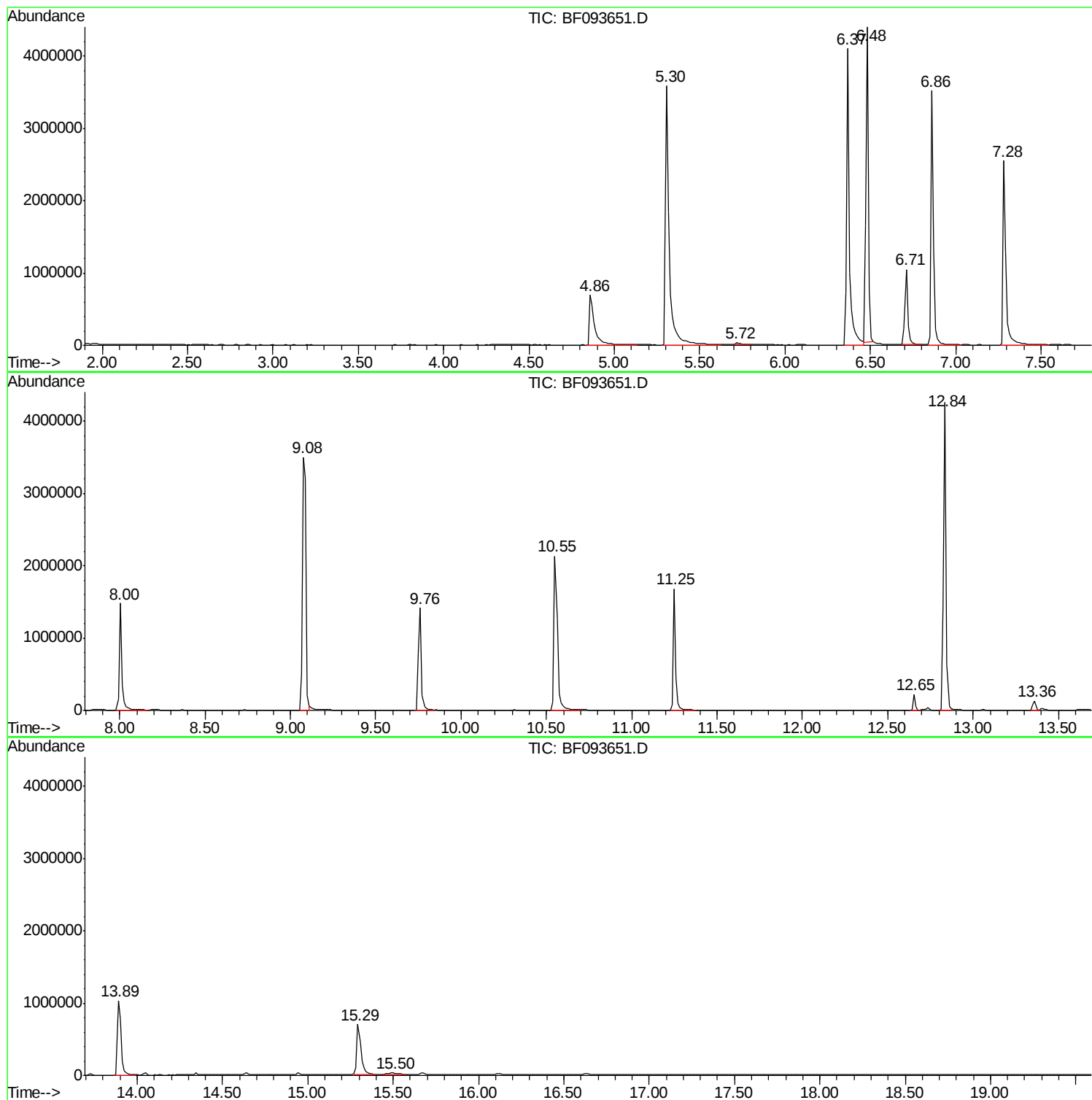
Sum of corrected areas: 44398646

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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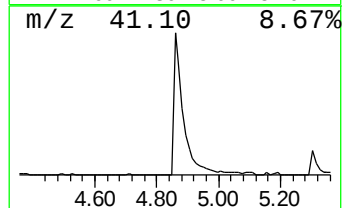
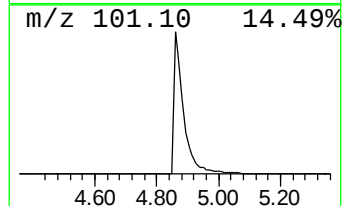
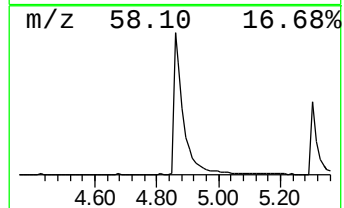
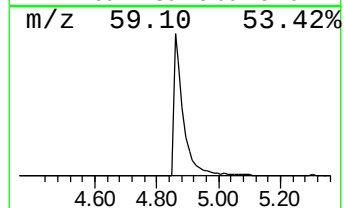
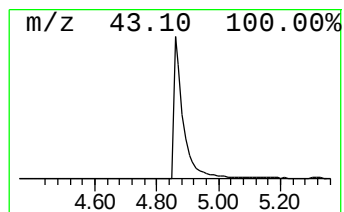
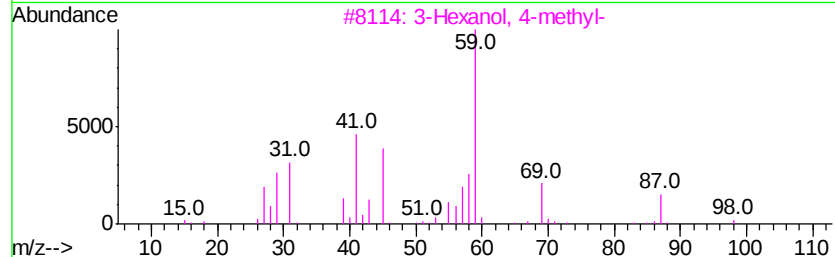
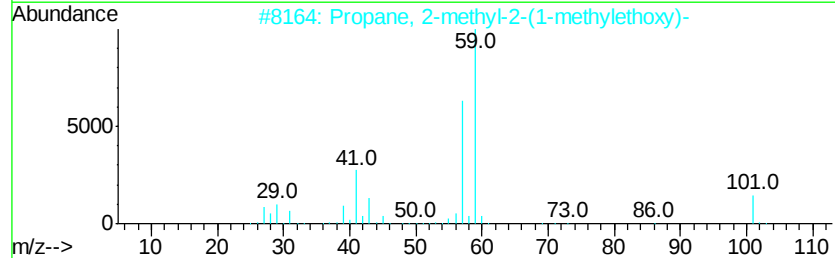
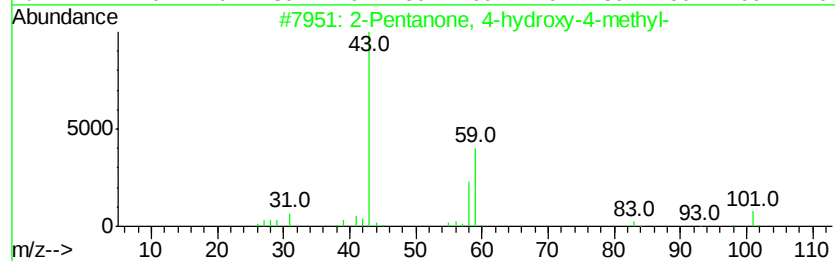
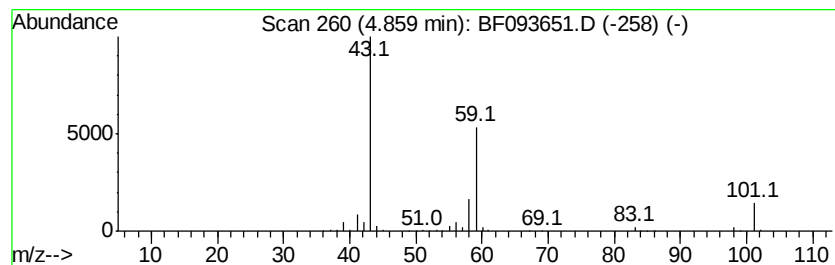
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	26.51 ng	1503610	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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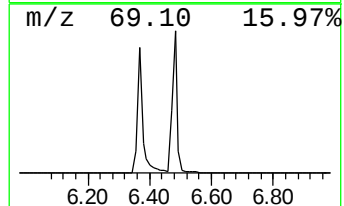
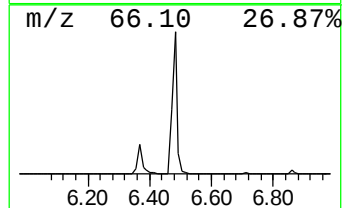
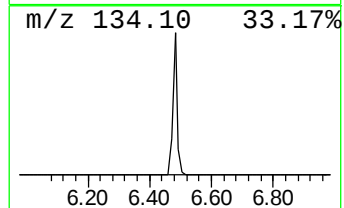
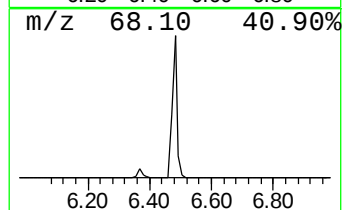
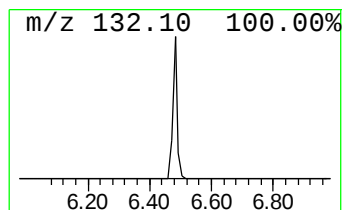
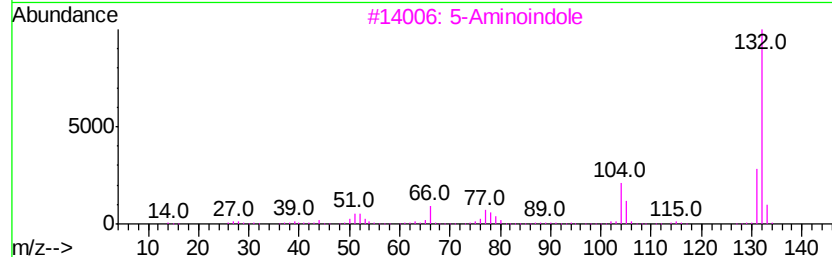
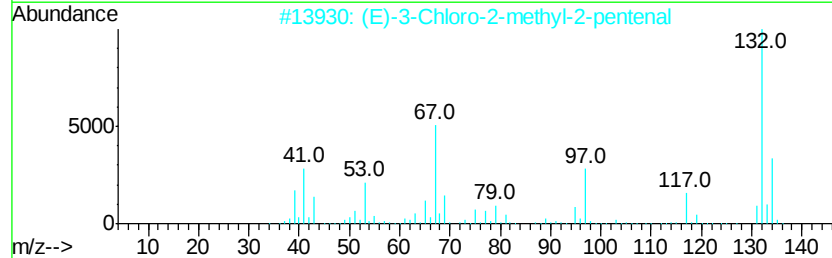
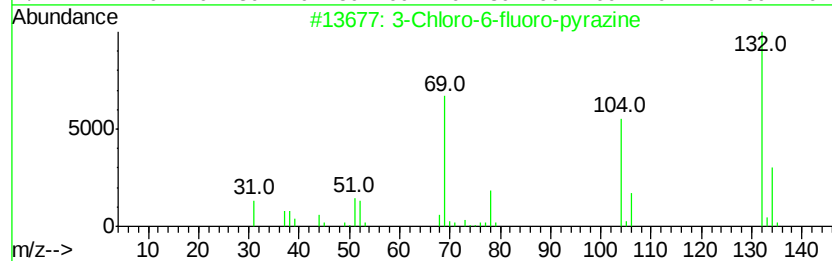
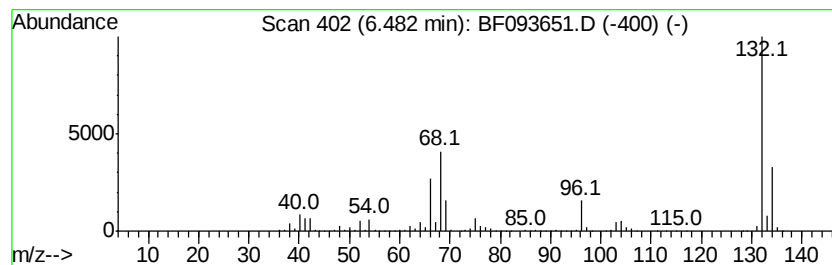
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Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	81.63 ng	4630300	1,4-Dichlorobenzene-d4	6.71

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	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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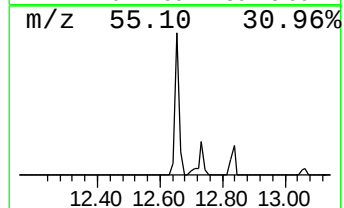
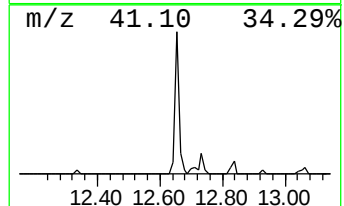
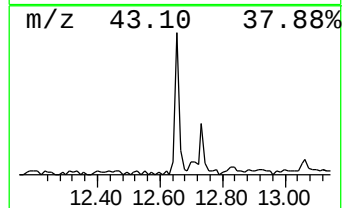
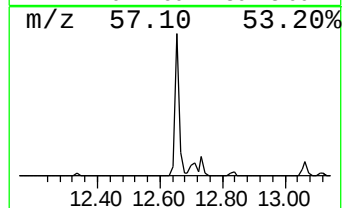
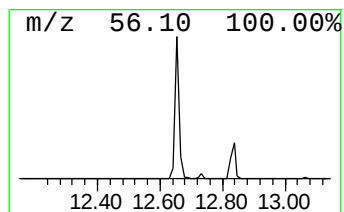
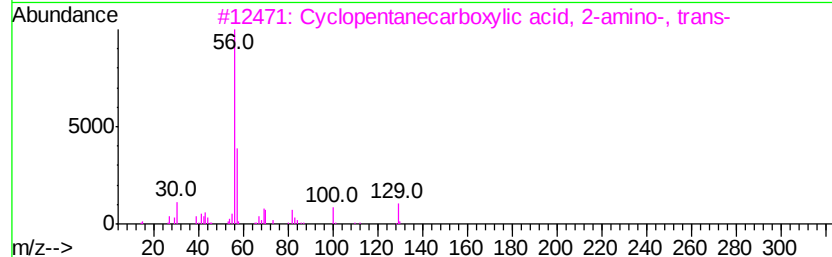
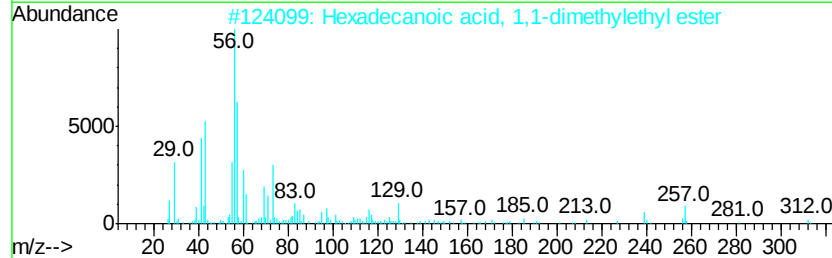
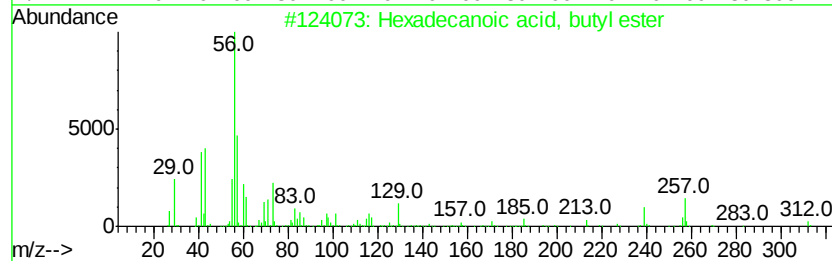
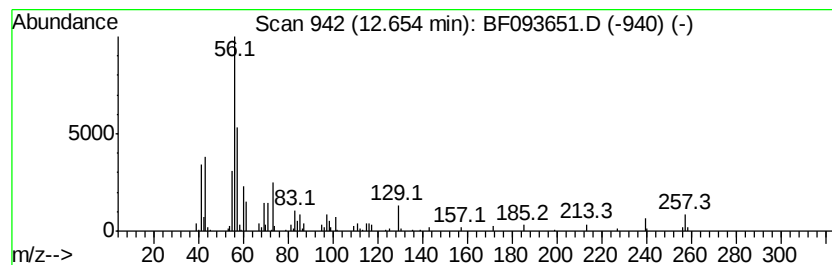
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.61 ng	190414	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	86
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	46
3		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
4		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	38
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.86	26.5	ng	1503610	1	6.71	1134510	20.0
unknown6.48	6.48	81.6	ng	4630300	1	6.71	1134510	20.0
Hexadecanoic acid...	12.65	2.6	ng	190414	5	13.89	1461030	20.0