

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052216\
 Data File : BF087298.D
 Acq On : 22 May 2016 18:44
 Operator : UM/SJ
 Sample : H3172-15
 Misc :
 ALS Vial : 66 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-12

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-BF051716.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	1.701	8	10	70	rVB	3806574	8253852	100.00%	21.152%
2	5.141	309	311	330	rBV	1529290	2027181	24.56%	5.195%
3	6.227	405	406	413	rBV	1120638	1400061	16.96%	3.588%
4	6.330	413	415	420	rVV	3642123	3726635	45.15%	9.550%
5	6.559	432	435	441	rVB	612185	778507	9.43%	1.995%
6	6.707	446	448	451	rBV	3344741	3142292	38.07%	8.053%
7	7.130	483	485	488	rBV	2129564	2782869	33.72%	7.132%
8	7.839	545	547	558	rBV2	745155	1050249	12.72%	2.691%
9	8.925	639	642	644	rBV	5168697	5010222	60.70%	12.839%
10	9.588	698	700	703	rBV	1277356	1137150	13.78%	2.914%
11	10.376	767	769	772	rBV2	2253632	2754187	33.37%	7.058%
12	11.062	827	829	832	rBV	934327	1052511	12.75%	2.697%
13	12.479	951	953	956	rVB	369108	309453	3.75%	0.793%
14	12.651	965	968	970	rBV	4099120	3955242	47.92%	10.136%
15	13.177	1012	1014	1016	rBV	160830	179309	2.17%	0.460%
16	13.691	1057	1059	1066	rBV	713198	782089	9.48%	2.004%
17	15.051	1175	1178	1187	rBV	411773	680400	8.24%	1.744%

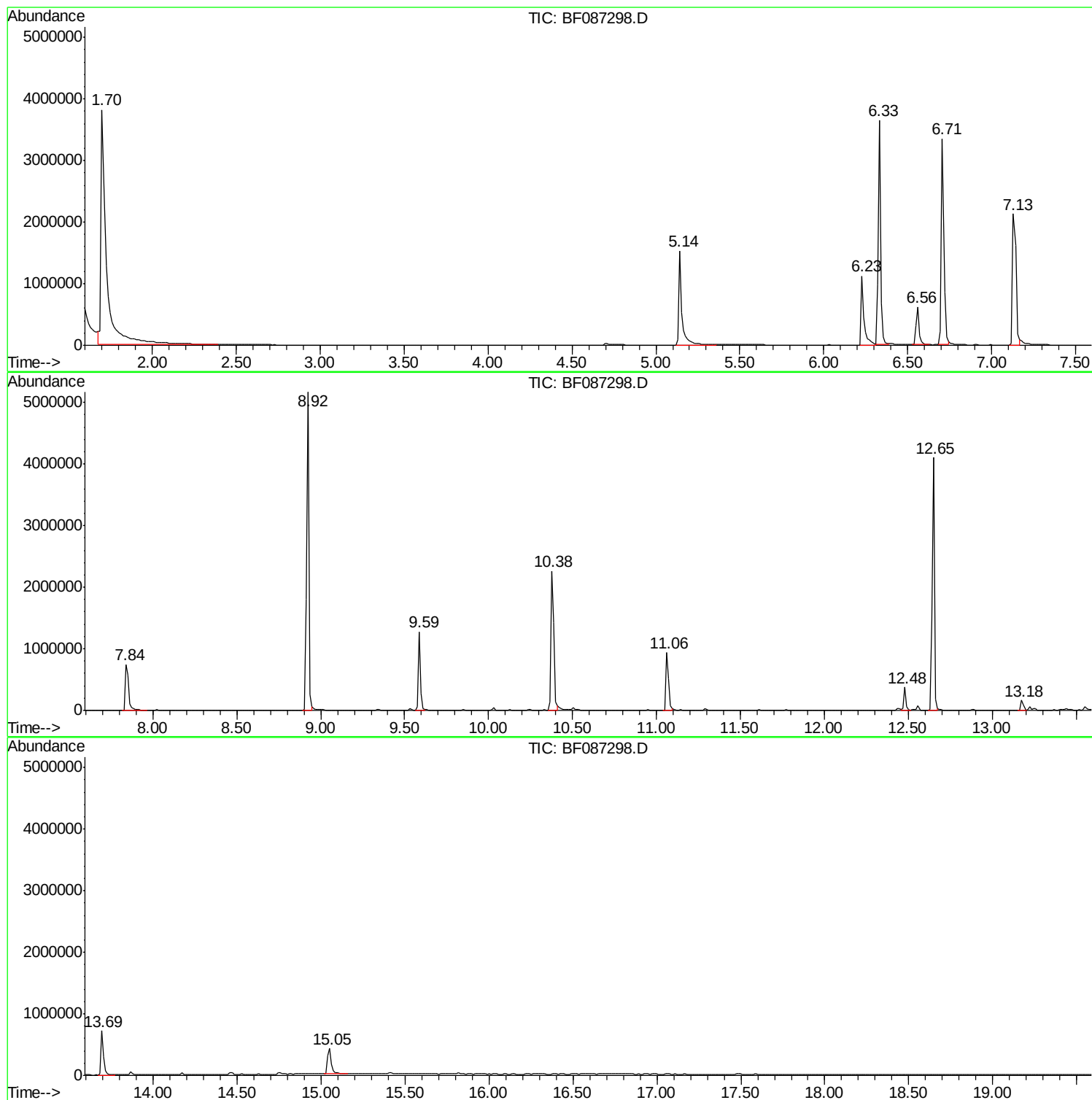
Sum of corrected areas: 39022209

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.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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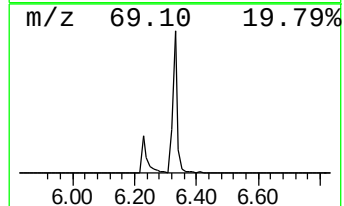
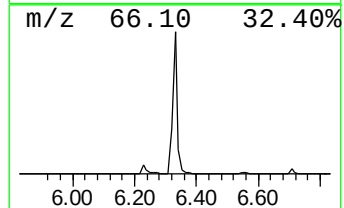
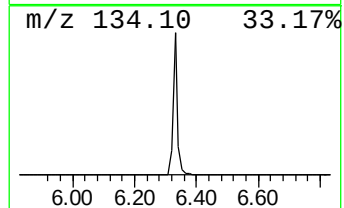
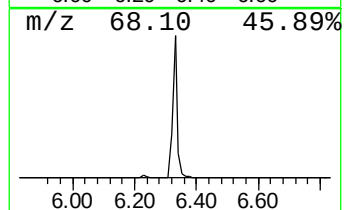
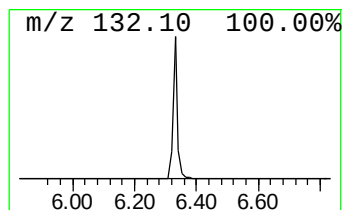
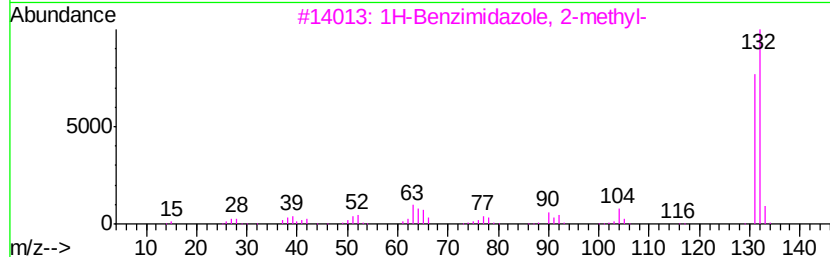
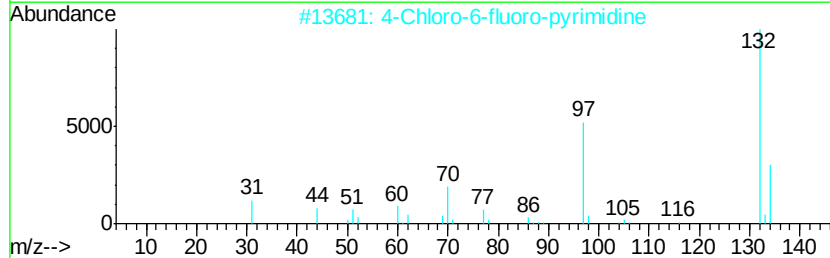
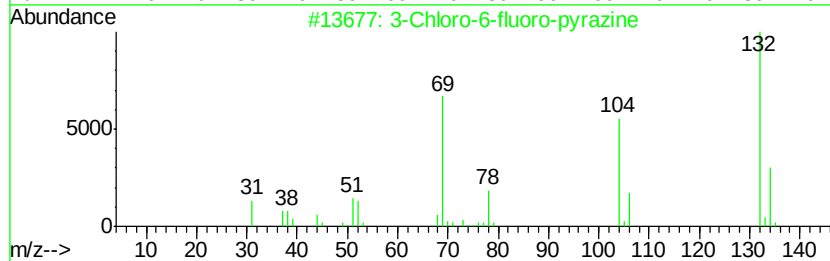
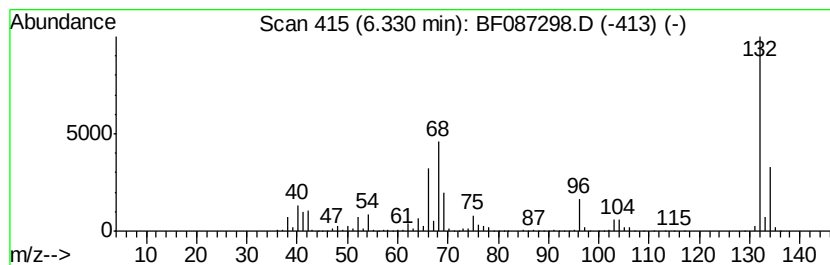
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.33 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	95.74 ng	3726640	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10



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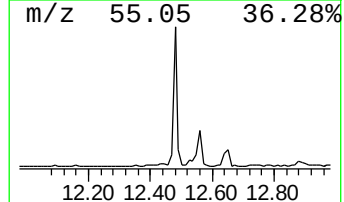
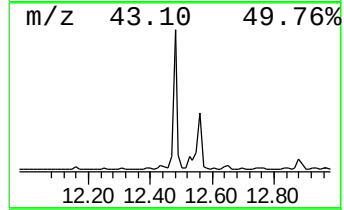
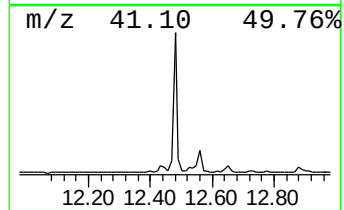
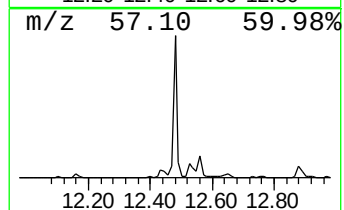
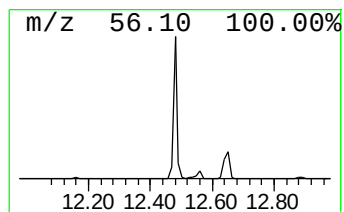
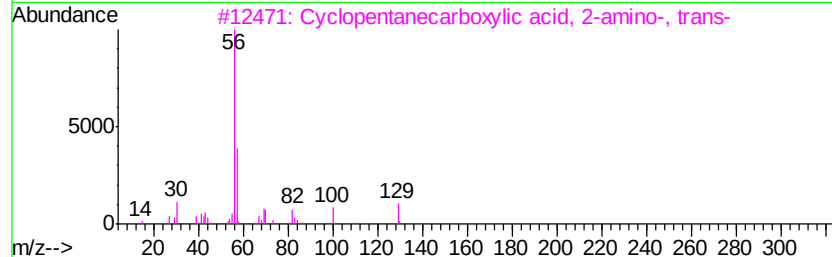
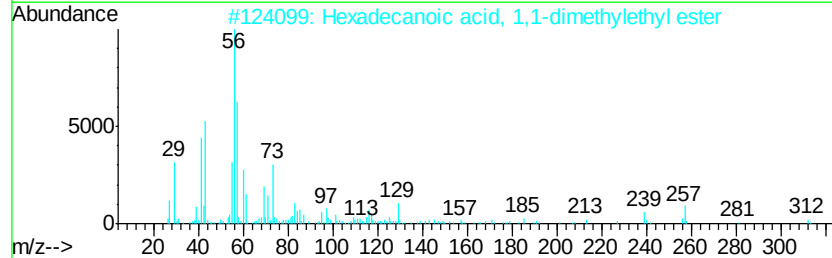
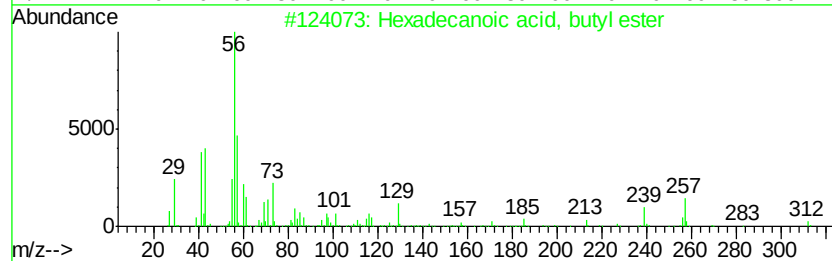
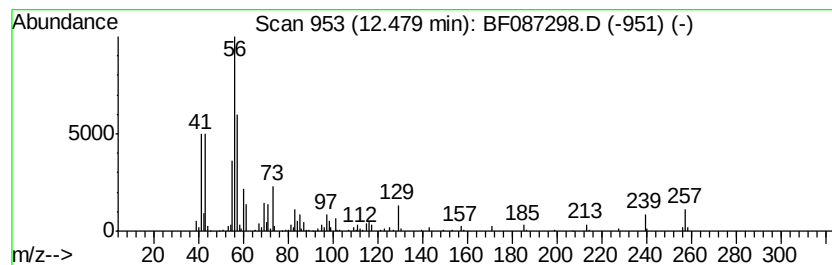
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	7.91 ng	309453	Chrysene-d12	13.69

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	52
3		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	37
4		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35
5		Cyclobutanone, 3,3-dimethyl-	98	C6H10O	001192-33-2	35



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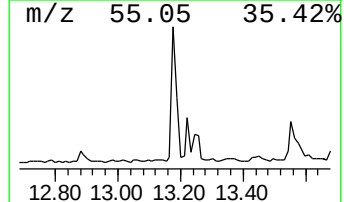
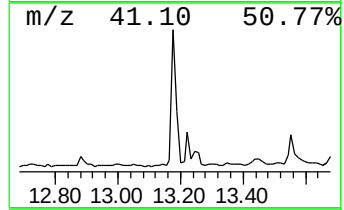
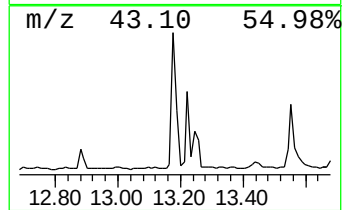
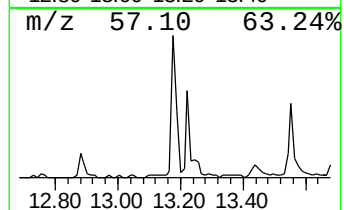
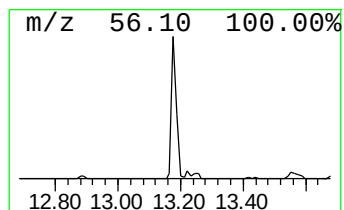
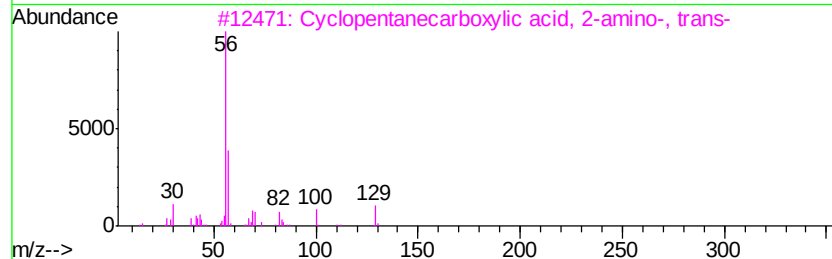
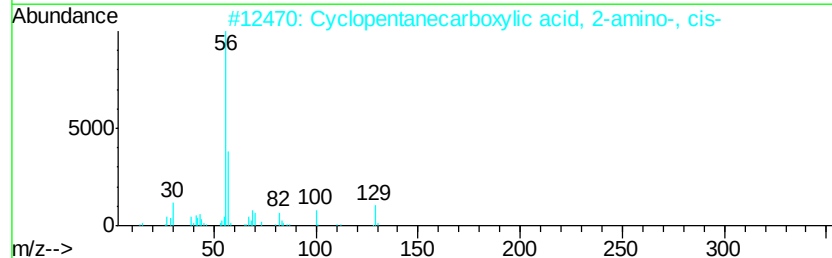
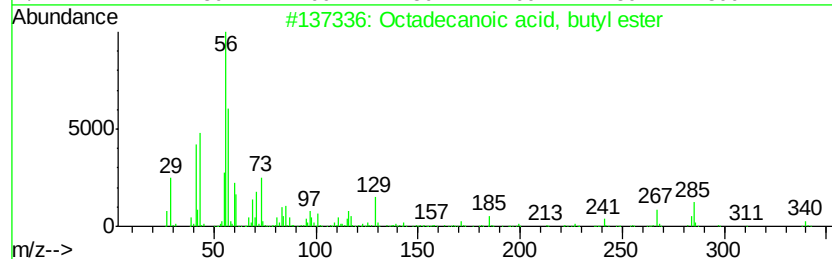
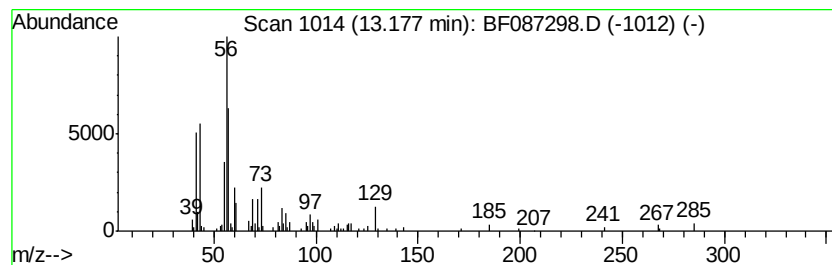
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Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.18	4.59 ng	179309	Chrysene-d12	13.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		Cyclopentanecarboxylic acid, 2-amino-, cis-	129	C6H11NO2	037910-65-9	46
3		Cyclopentanecarboxylic acid, 2-amino-, trans-	129	C6H11NO2	040482-05-1	43
4		1-Hexanol, 3,5,5-trimethyl-	144	C9H20O	003452-97-9	38
5		Cyclohexanol, 2-amino-, trans-	115	C6H13NO	006982-39-4	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.33	6.33	95.7	ng	3726640	1	6.56	778507	20.0
Hexadecanoic acid...	12.48	7.9	ng	309453	5	13.69	782089	20.0
Octadecanoic acid...	13.18	4.6	ng	179309	5	13.69	782089	20.0