

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081716\
 Data File : BF089761.D
 Acq On : 17 Aug 2016 14:29
 Operator : UM/SJ
 Sample : H4476-06
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LOCATION-46A

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-BF081616.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	1.667	6	7	16	rVV	1870050	3179628	8.56%	1.672%
2	1.793	16	18	64	rVB	13757863	37162332	100.00%	19.537%
3	4.844	282	285	296	rVB	1220984	1704616	4.59%	0.896%
4	5.279	320	323	325	rBV	8660885	8666277	23.32%	4.556%
5	6.330	412	415	417	rBV	5899730	5776144	15.54%	3.037%
6	6.467	424	427	429	rBV	13752624	16211536	43.62%	8.523%
7	6.696	445	447	449	rBV	4854737	4127941	11.11%	2.170%
8	6.856	458	461	463	rBV	14590241	13724542	36.93%	7.215%
9	7.267	493	497	499	rBV	10454213	11860634	31.92%	6.235%
10	7.988	557	560	562	rVB	5567510	5874188	15.81%	3.088%
11	9.073	651	655	657	rVB	18740603	22527642	60.62%	11.843%
12	9.462	686	689	691	rBV	487152	435317	1.17%	0.229%
13	9.736	710	713	715	rBV	7718191	6825719	18.37%	3.588%
14	10.525	778	782	784	rBV	11058660	13464379	36.23%	7.079%
15	11.211	839	842	844	rBV	7735439	6567767	17.67%	3.453%
16	11.759	888	890	892	rBV	538032	597007	1.61%	0.314%
17	12.548	957	959	965	rVV	695626	828425	2.23%	0.436%
18	12.651	965	968	970	rVB	633843	757321	2.04%	0.398%
19	12.811	979	982	984	rBV	15345196	18482646	49.73%	9.717%
20	13.371	1029	1031	1033	rBV	394939	571891	1.54%	0.301%
21	13.874	1072	1075	1078	rBV	5661552	6023313	16.21%	3.167%
22	15.348	1201	1204	1207	rBV	3180231	4843024	13.03%	2.546%

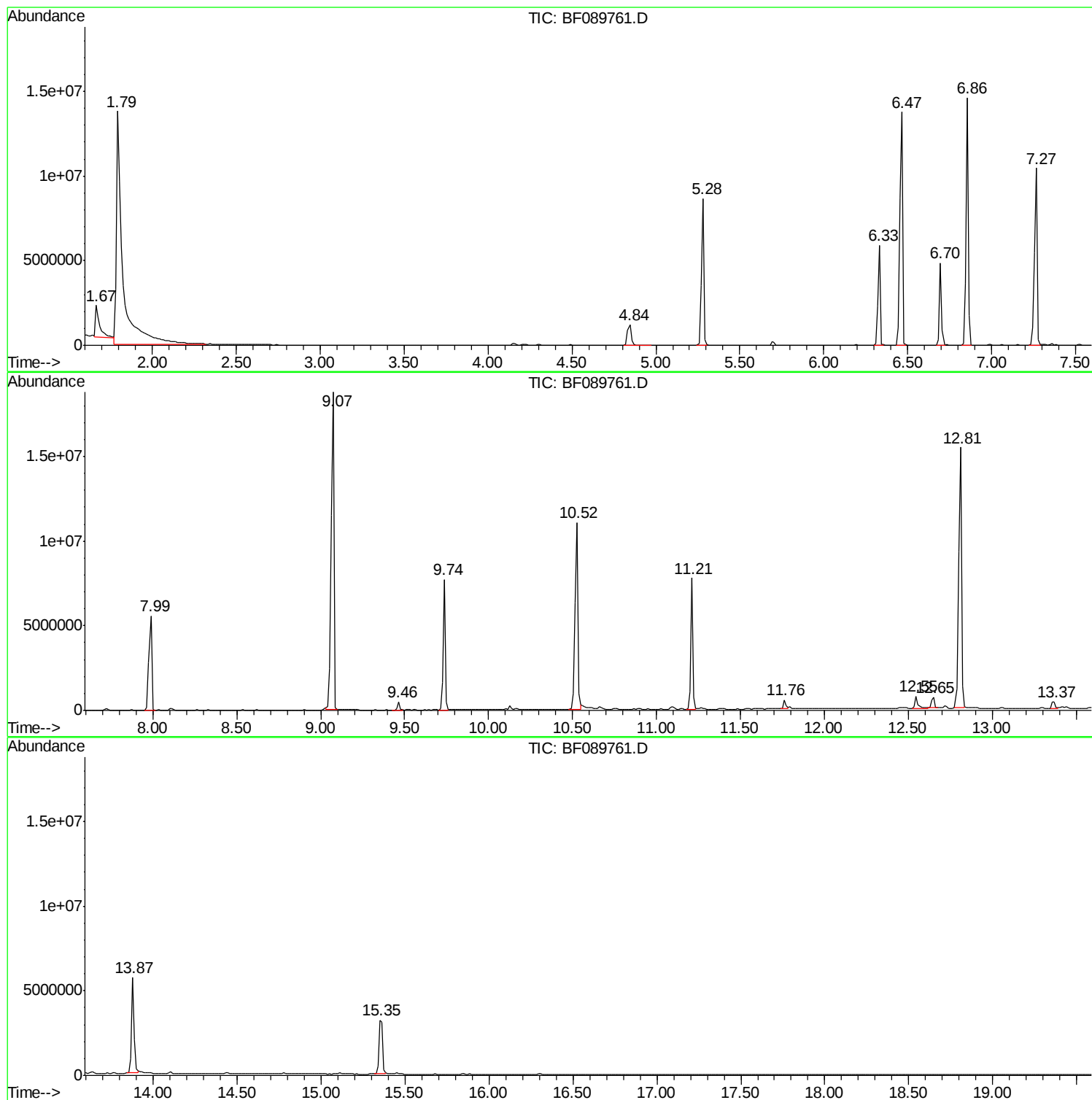
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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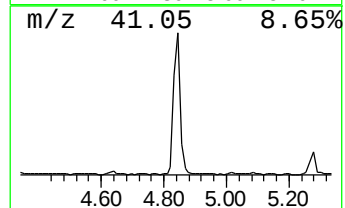
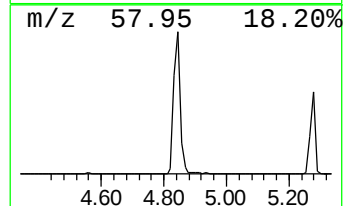
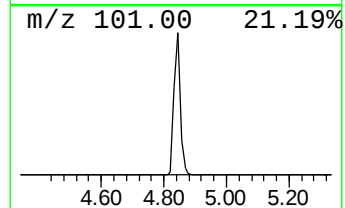
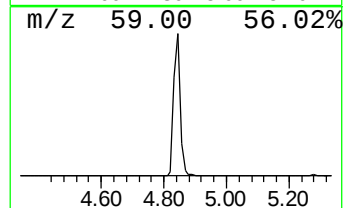
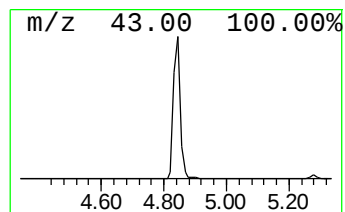
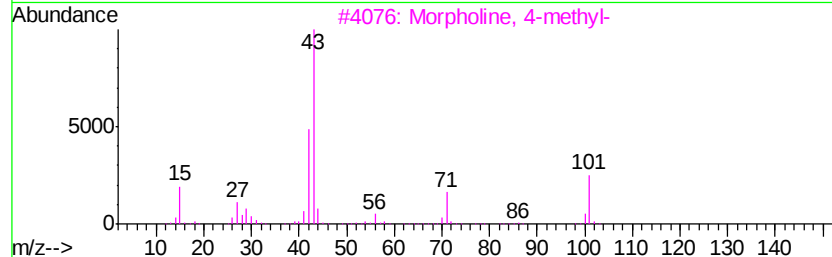
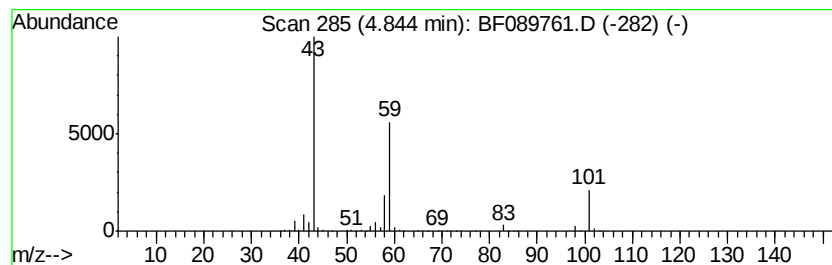
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	8.26 ng	1704620	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Acetone	58	C3H6O	000067-64-1	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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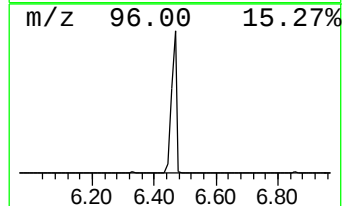
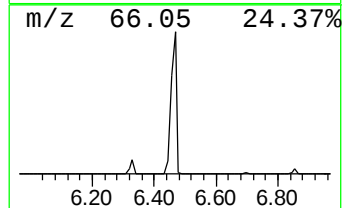
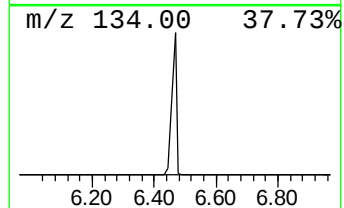
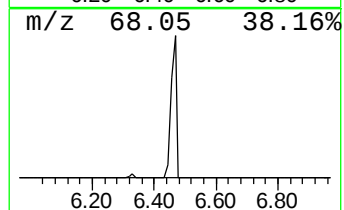
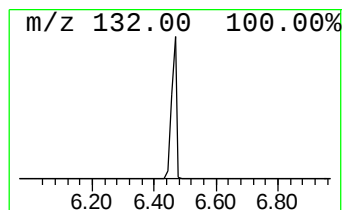
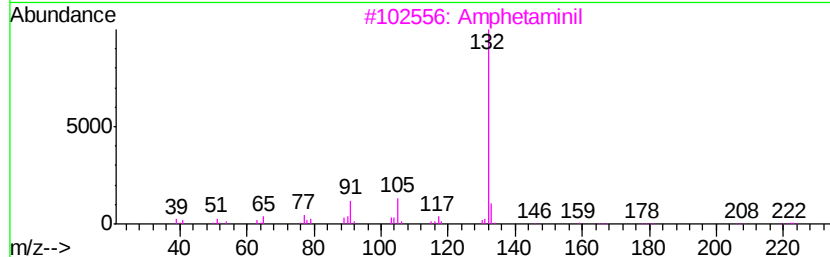
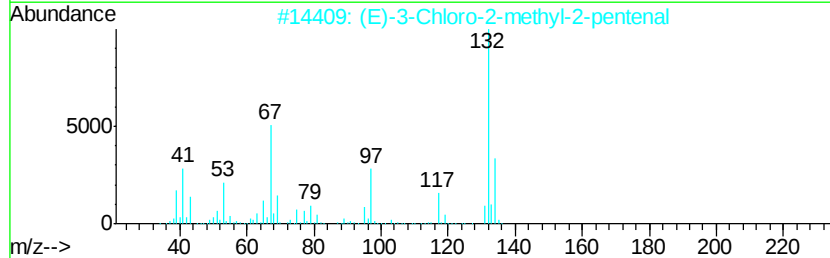
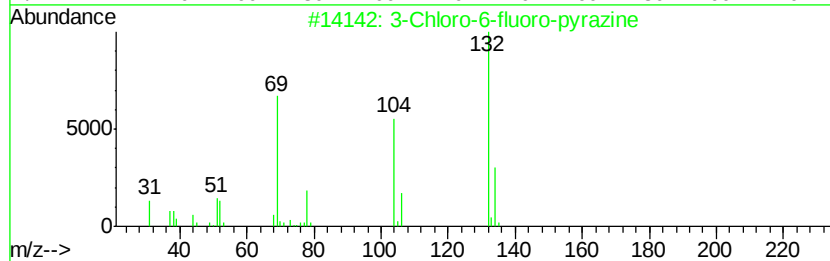
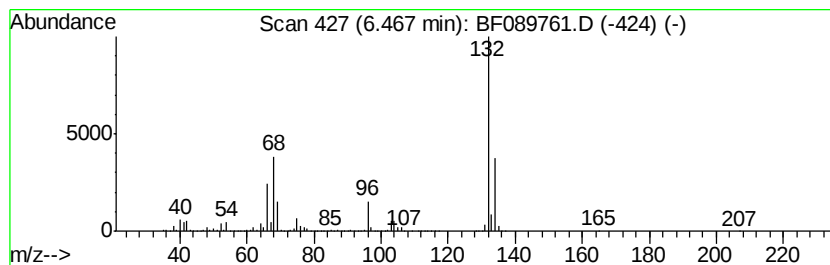
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Peak Number 4 unknown6.47 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	78.55 ng	16211500	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		Amphetaminil	250	C17H18N2	017590-01-1	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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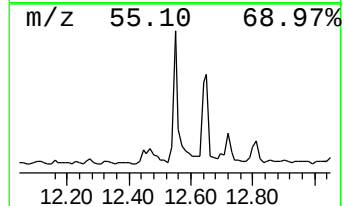
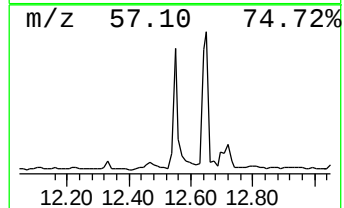
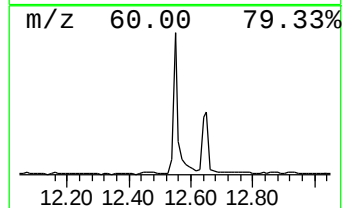
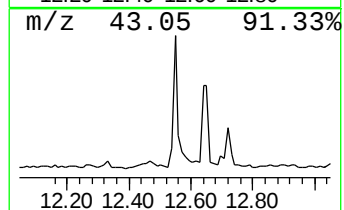
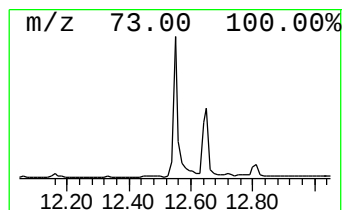
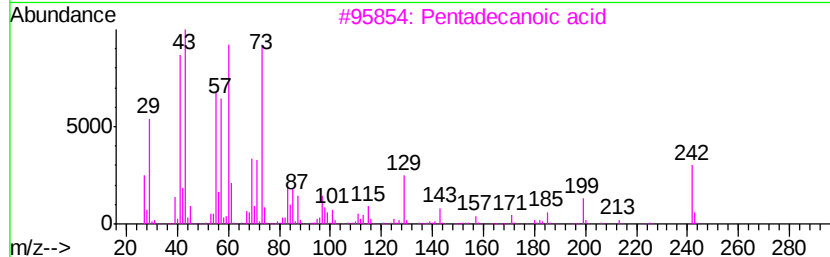
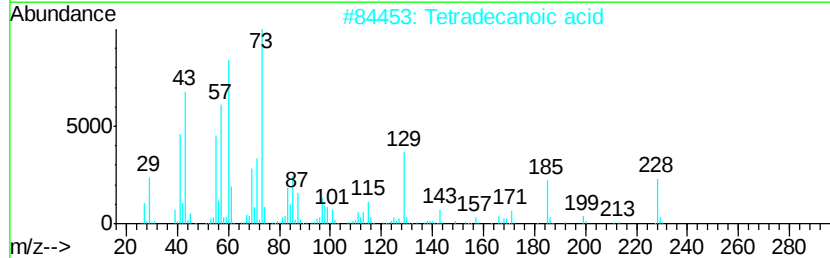
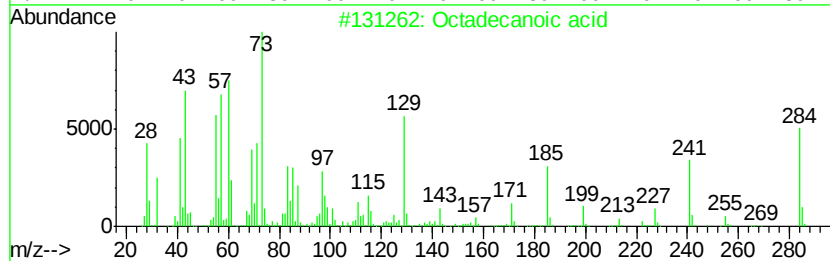
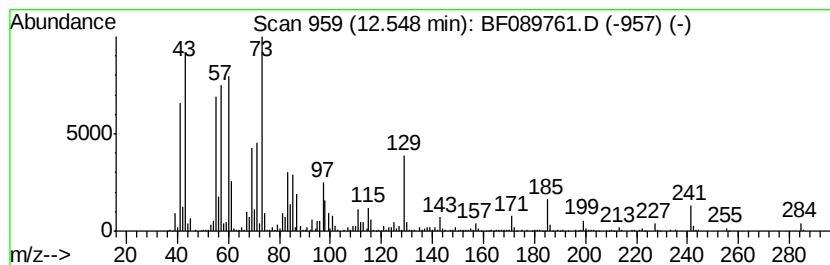
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Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	2.75 ng	828425	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4		n-Decanoic acid	172	C10H20O2	000334-48-5	68
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	45



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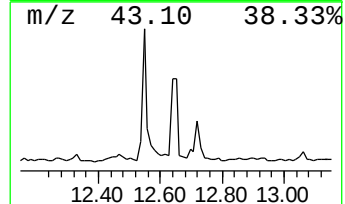
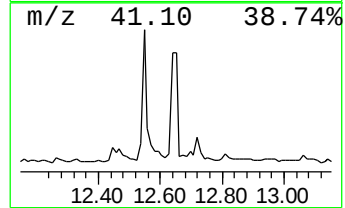
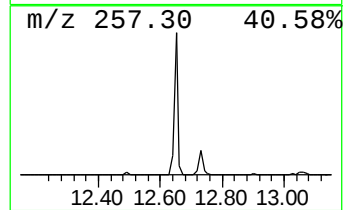
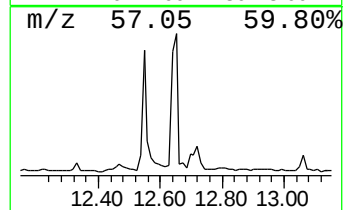
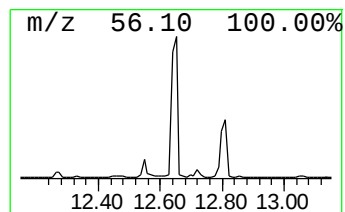
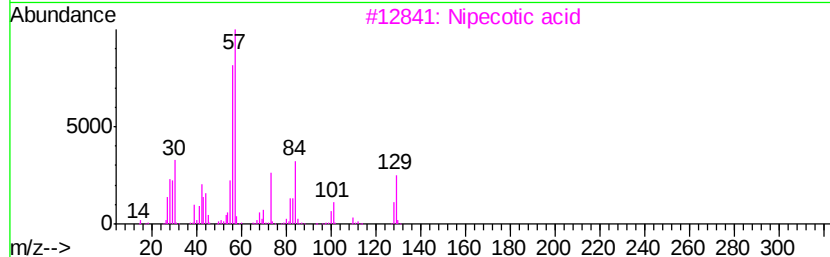
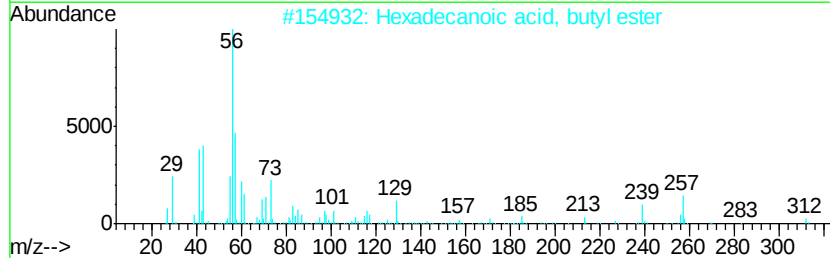
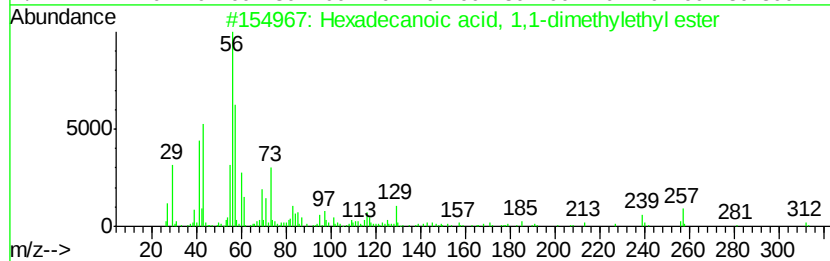
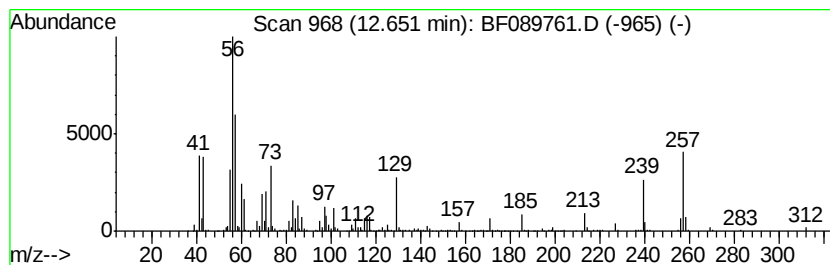
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Peak Number 7 Hexadecanoic acid, 1,1-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.51 ng	757321	Chrysene-d12	13.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	96
2			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3			Nipecotic acid	129	C6H11NO2	000498-95-3	43
4			Hexadecanoic acid, 2-methylpropv...	312	C20H40O2	000110-34-9	38
5			1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.84	8.3	ng	1704620	1	6.70	4127940	20.0
unknown6.47	6.47	78.5	ng	16211500	1	6.70	4127940	20.0
Octadecanoic acid	12.55	2.8	ng	828425	5	13.87	6023310	20.0
Hexadecanoic acid...	12.65	2.5	ng	757321	5	13.87	6023310	20.0