

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060117\
 Data File : BF095599.D
 Acq On : 1 Jun 2017 17:32
 Operator : SJ/MA
 Sample : I3379-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S22-0027

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-BF050217.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	2.281	97	101	112	rBV	32175	57903	1.72%	0.283%
2	4.792	525	528	539	rBV2	19118	52580	1.56%	0.257%
3	5.457	638	641	665	rBV	351366	929157	27.54%	4.539%
4	7.104	918	921	932	rBV	219471	529552	15.70%	2.587%
5	7.192	932	936	962	rVB	1378581	2325312	68.92%	11.359%
6	7.533	991	994	1007	rBV	382681	538371	15.96%	2.630%
7	7.775	1029	1035	1048	rBV	1413939	1990315	58.99%	9.722%
8	8.451	1145	1150	1167	rBV	1087508	1638754	48.57%	8.005%
9	8.922	1224	1230	1238	rBV	36145	56694	1.68%	0.277%
10	9.569	1336	1340	1361	rBV	489604	708633	21.00%	3.462%
11	10.410	1476	1483	1489	rBV	38770	56224	1.67%	0.275%
12	11.345	1635	1642	1656	rBV	2439025	3373876	100.00%	16.481%
13	12.045	1757	1761	1768	rBV	51376	70891	2.10%	0.346%
14	12.392	1815	1820	1834	rBV2	629241	837848	24.83%	4.093%
15	13.692	2036	2041	2057	rBV	1196812	1739349	51.55%	8.496%
16	14.798	2224	2229	2241	rBV	585649	796472	23.61%	3.891%
17	15.786	2391	2397	2407	rBV2	93348	131642	3.90%	0.643%
18	16.880	2577	2583	2593	rBV	67605	98493	2.92%	0.481%
19	17.150	2623	2629	2633	rBV2	2444239	3064516	90.83%	14.970%
20	18.392	2836	2840	2847	rBV3	48725	75617	2.24%	0.369%
21	18.492	2853	2857	2871	rVB	562693	789237	23.39%	3.855%
22	20.168	3138	3142	3155	rBV	407143	610185	18.09%	2.981%

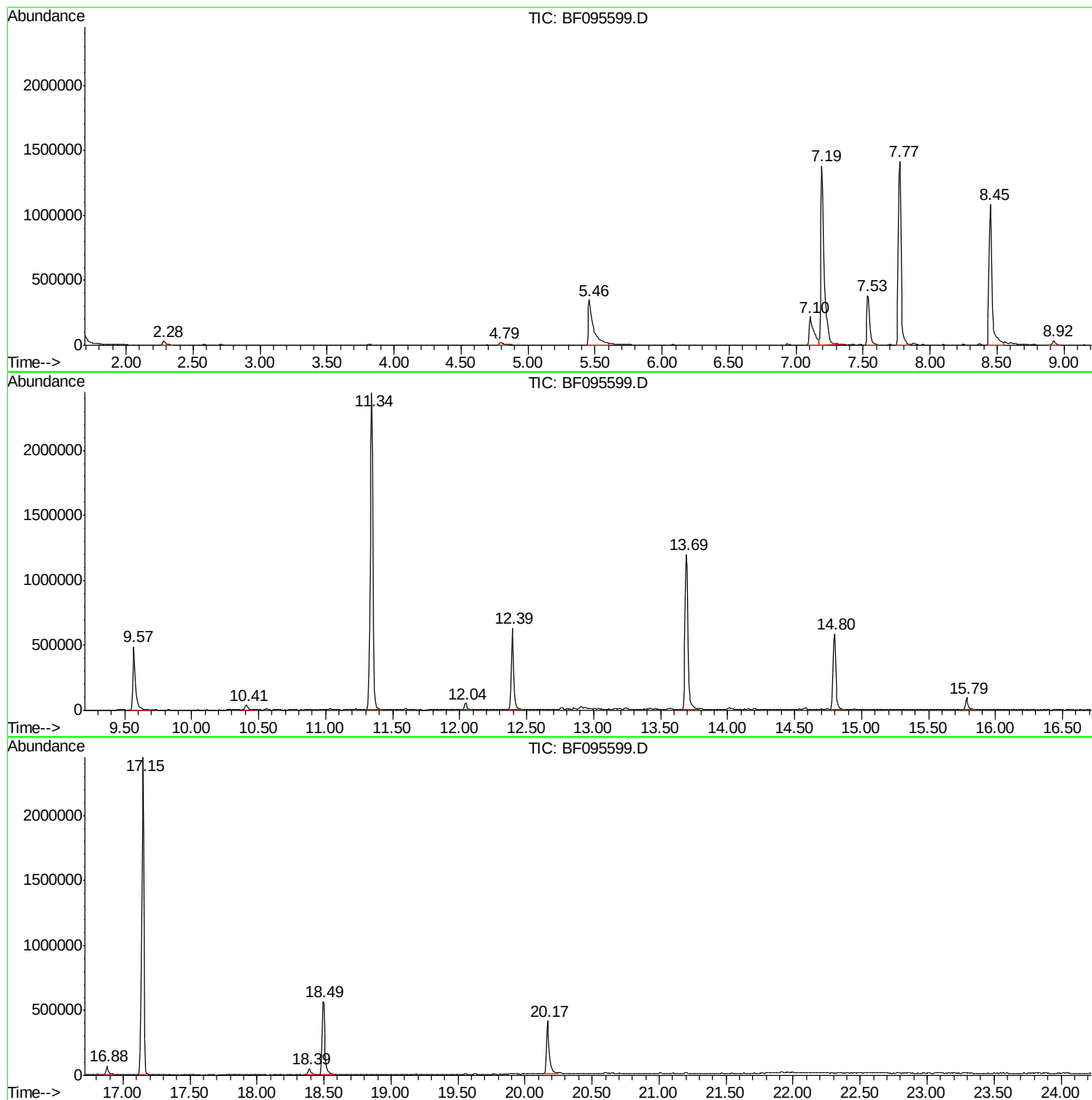
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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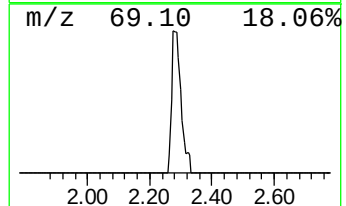
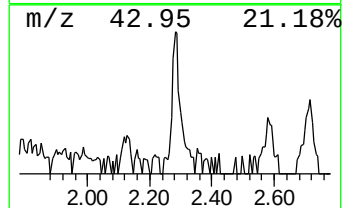
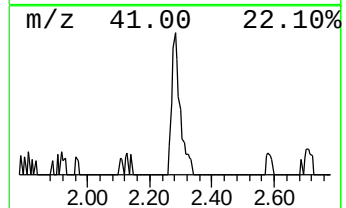
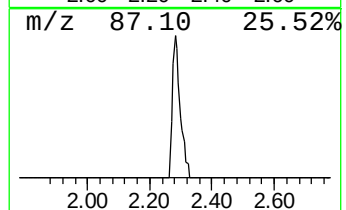
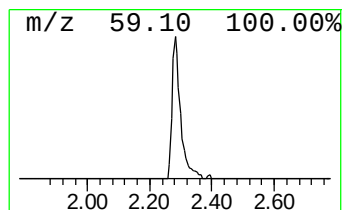
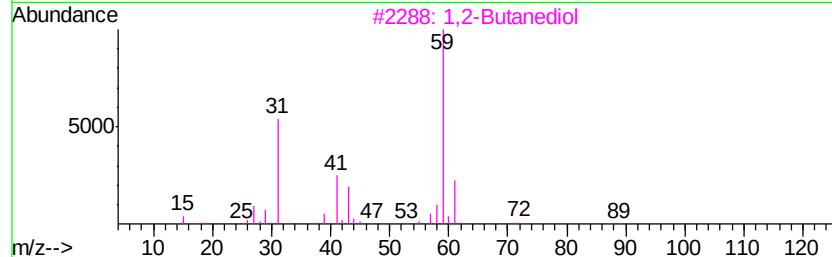
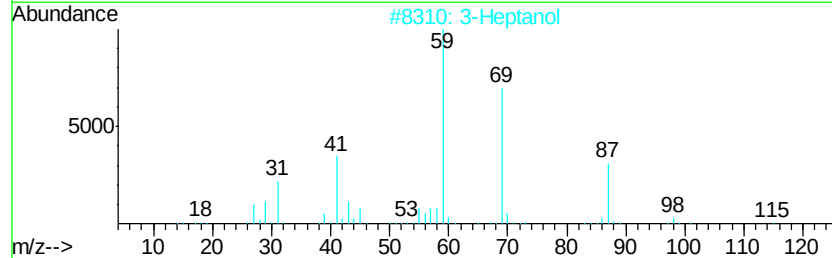
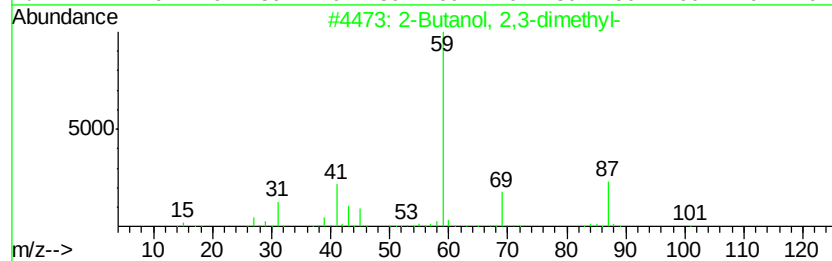
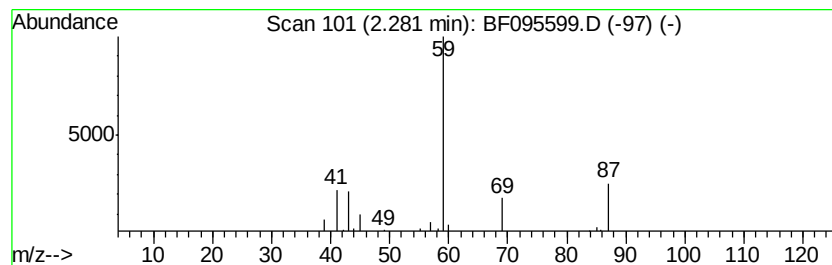
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Butanol, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.28	2.15 ng	57903	1,4-Dichlorobenzene-d4	7.53

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2			3-Heptanol	116	C7H16O	000589-82-2	40
3			1,2-Butanediol	90	C4H10O2	000584-03-2	33
4			Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	33
5			3-Pentanol	88	C5H12O	000584-02-1	33



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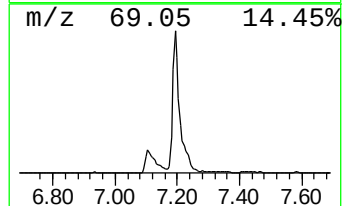
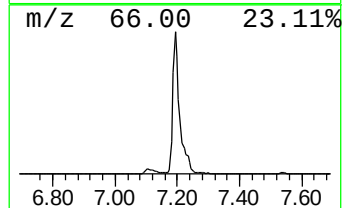
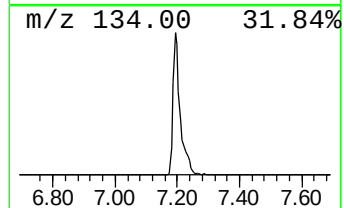
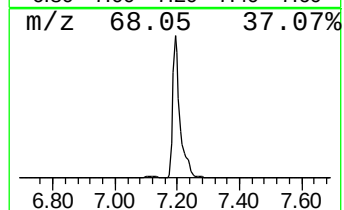
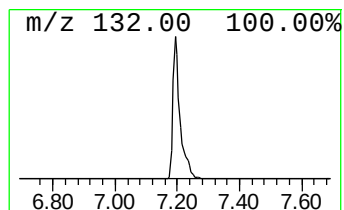
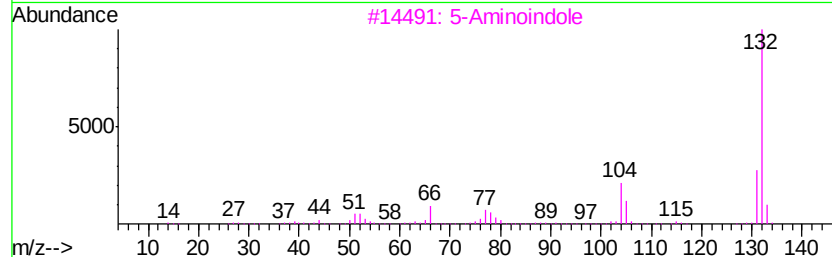
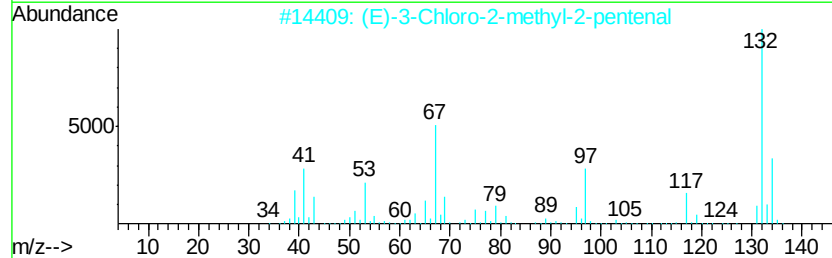
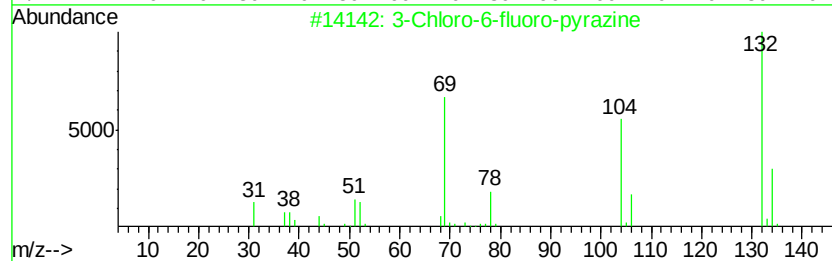
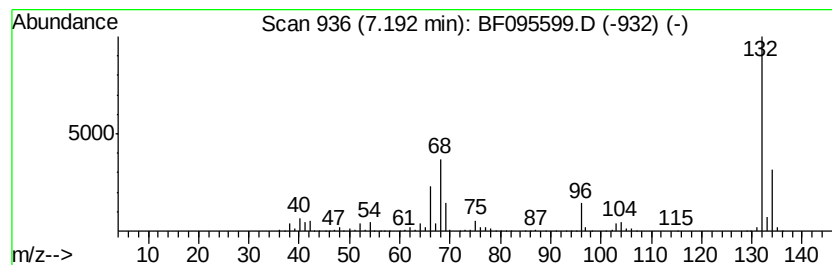
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Peak Number 2 unknown7.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	86.38 ng	2325310	1,4-Dichlorobenzene-d4	7.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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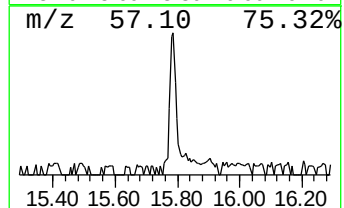
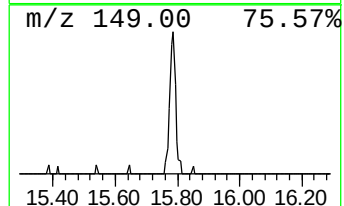
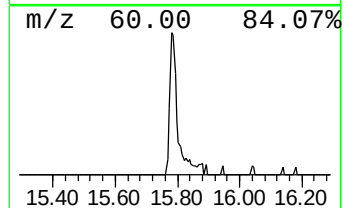
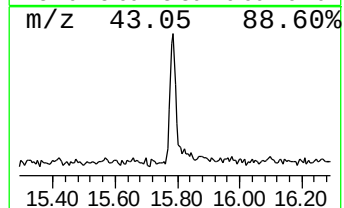
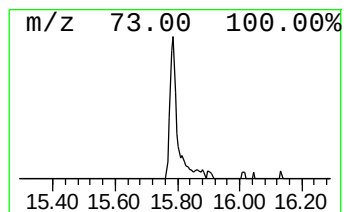
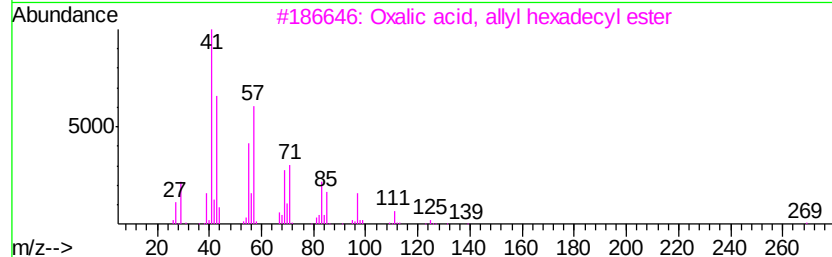
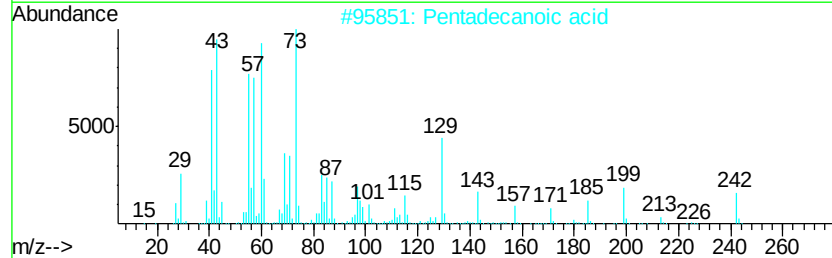
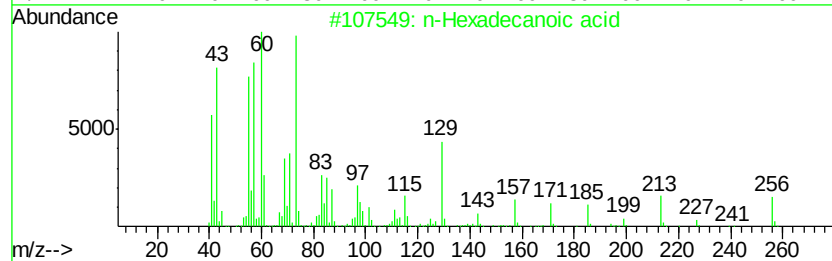
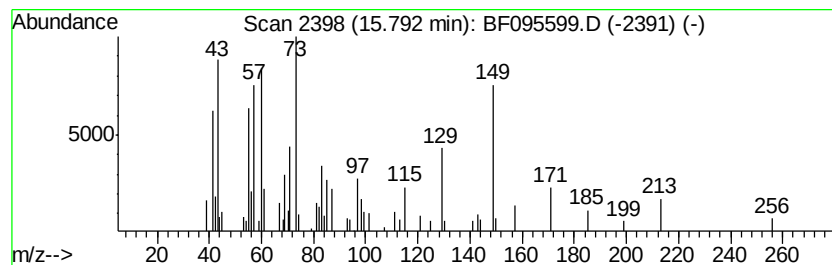
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	3.31 ng	131642	Phenanthrene-d10	14.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	62
3		Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20
4		Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1000309-70-5	18
5		Oxalic acid, allyl tridecyl ester	312	C18H32O4	1000309-24-1	18



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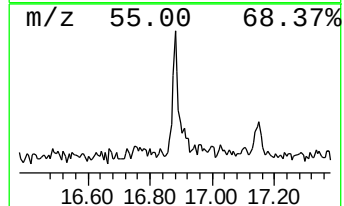
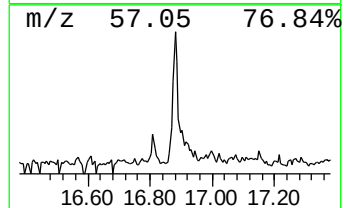
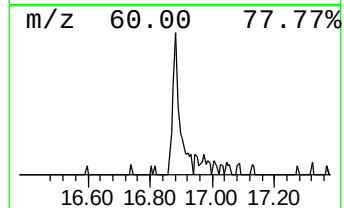
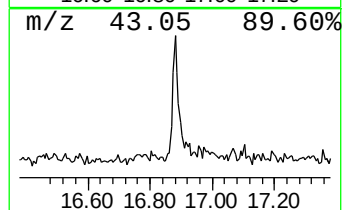
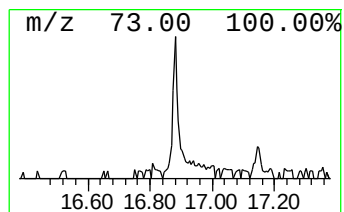
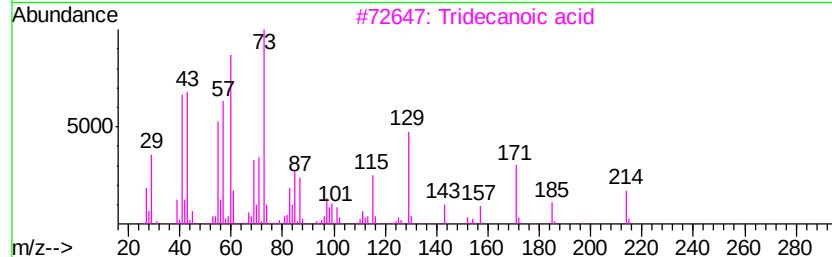
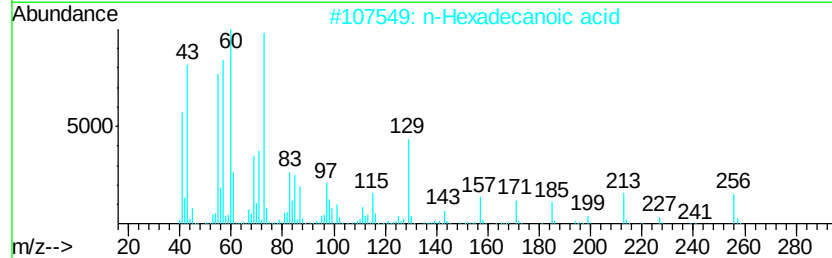
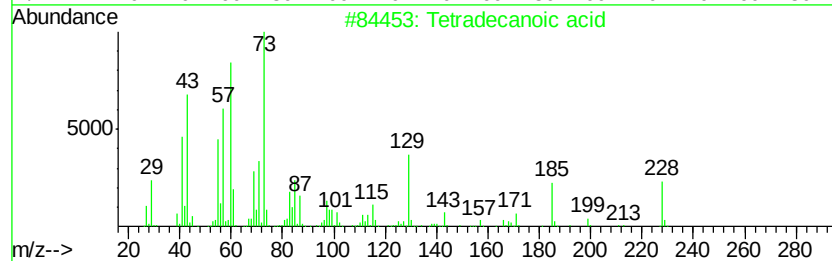
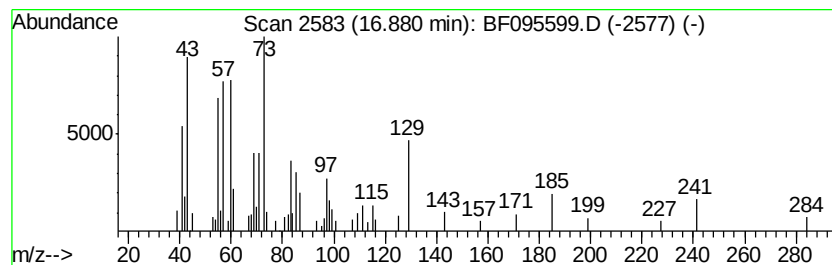
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Peak Number 5 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.88	2.50 ng	98493	Chrysene-d12	18.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
3		Tridecanoic acid	214	C13H26O2	000638-53-9	72
4		Octadecanoic acid	284	C18H36O2	000057-11-4	62
5		n-Decanoic acid	172	C10H20O2	000334-48-5	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Butanol, 2,3-di...	2.28	2.1	ng	57903	1	7.53	538371	20.0
unknown7.19	7.19	86.4	ng	2325310	1	7.53	538371	20.0
n-Hexadecanoic acid	15.79	3.3	ng	131642	4	14.80	796472	20.0
Tetradecanoic acid	16.88	2.5	ng	98493	5	18.50	789237	20.0