

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
 Data File : BF095578.D
 Acq On : 31 May 2017 22:49
 Operator : SJ/MA
 Sample : I3341-04
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NM14-COMP-6-18

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-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	4.790	498	502	512	rBV	56791	133641	6.81%	0.769%
2	5.460	613	616	642	rBV	776572	1729827	88.20%	9.949%
3	7.101	892	895	910	rBV	941456	1696225	86.48%	9.756%
4	7.213	910	914	930	rVB	1135197	1801067	91.83%	10.359%
5	7.554	968	972	982	rBV	392270	504143	25.70%	2.900%
6	7.789	1007	1012	1025	rBV	938932	1201495	61.26%	6.910%
7	8.466	1122	1127	1159	rBV	594016	967184	49.31%	5.563%
8	9.583	1313	1317	1331	rBV	518729	699394	35.66%	4.023%
9	11.007	1554	1559	1566	rBV4	7922	23150	1.18%	0.133%
10	11.360	1614	1619	1632	rBV	1606402	1961310	100.00%	11.281%
11	12.048	1732	1736	1748	rBV	229811	296950	15.14%	1.708%
12	12.407	1792	1797	1812	rBV2	587107	771975	39.36%	4.440%
13	13.254	1935	1941	1945	rBV	31249	37096	1.89%	0.213%
14	13.707	2013	2018	2035	rBV	622504	939072	47.88%	5.401%
15	14.024	2067	2072	2075	rBV	31550	38311	1.95%	0.220%
16	14.760	2193	2197	2201	rBV	23220	26881	1.37%	0.155%
17	14.813	2201	2206	2210	rVV	502409	648980	33.09%	3.733%
18	14.848	2210	2212	2218	rVB	55231	81161	4.14%	0.467%
19	14.948	2226	2229	2238	rVB	16154	26037	1.33%	0.150%
20	15.424	2306	2310	2317	rBV4	11842	19714	1.01%	0.113%
21	15.795	2370	2373	2383	rVB2	112291	155110	7.91%	0.892%
22	16.612	2509	2512	2516	rVV	146165	157546	8.03%	0.906%
23	16.695	2523	2526	2533	rBV8	25230	41761	2.13%	0.240%
24	16.801	2540	2544	2549	rVB5	29666	41159	2.10%	0.237%
25	16.912	2560	2563	2568	rVB	129714	157918	8.05%	0.908%
26	17.154	2600	2604	2609	rBV	980183	1142199	58.24%	6.569%
27	17.383	2640	2643	2648	rVB4	19887	32633	1.66%	0.188%
28	17.518	2662	2666	2669	rBV4	27064	39846	2.03%	0.229%
29	17.859	2720	2724	2727	rBV	29698	35330	1.80%	0.203%
30	18.136	2768	2771	2776	rBV6	30512	46390	2.37%	0.267%
31	18.359	2803	2809	2812	rBV7	17086	32037	1.63%	0.184%
32	18.406	2812	2817	2822	rBV3	94051	167266	8.53%	0.962%
33	18.506	2829	2834	2838	rBV	572519	713169	36.36%	4.102%
34	18.636	2852	2856	2859	rBV5	29923	42754	2.18%	0.246%

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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

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35	18.730	2871	2872	2876	rVB4	19426	22109	1.13%	0.127%
36	18.818	2881	2887	2890	rBV7	26698	53391	2.72%	0.307%
37	18.965	2908	2912	2914	rBV5	24655	38156	1.95%	0.219%
38	19.212	2950	2954	2955	rBV3	28837	37392	1.91%	0.215%
39	19.777	3047	3050	3054	rBV	94505	126764	6.46%	0.729%
40	20.071	3097	3100	3104	rVB	64029	64348	3.28%	0.370%
41	20.130	3107	3110	3114	rVV	85272	99894	5.09%	0.575%
42	20.177	3114	3118	3127	rVV	380529	505399	25.77%	2.907%
43	23.547	3688	3691	3694	rBV5	19428	30528	1.56%	0.176%

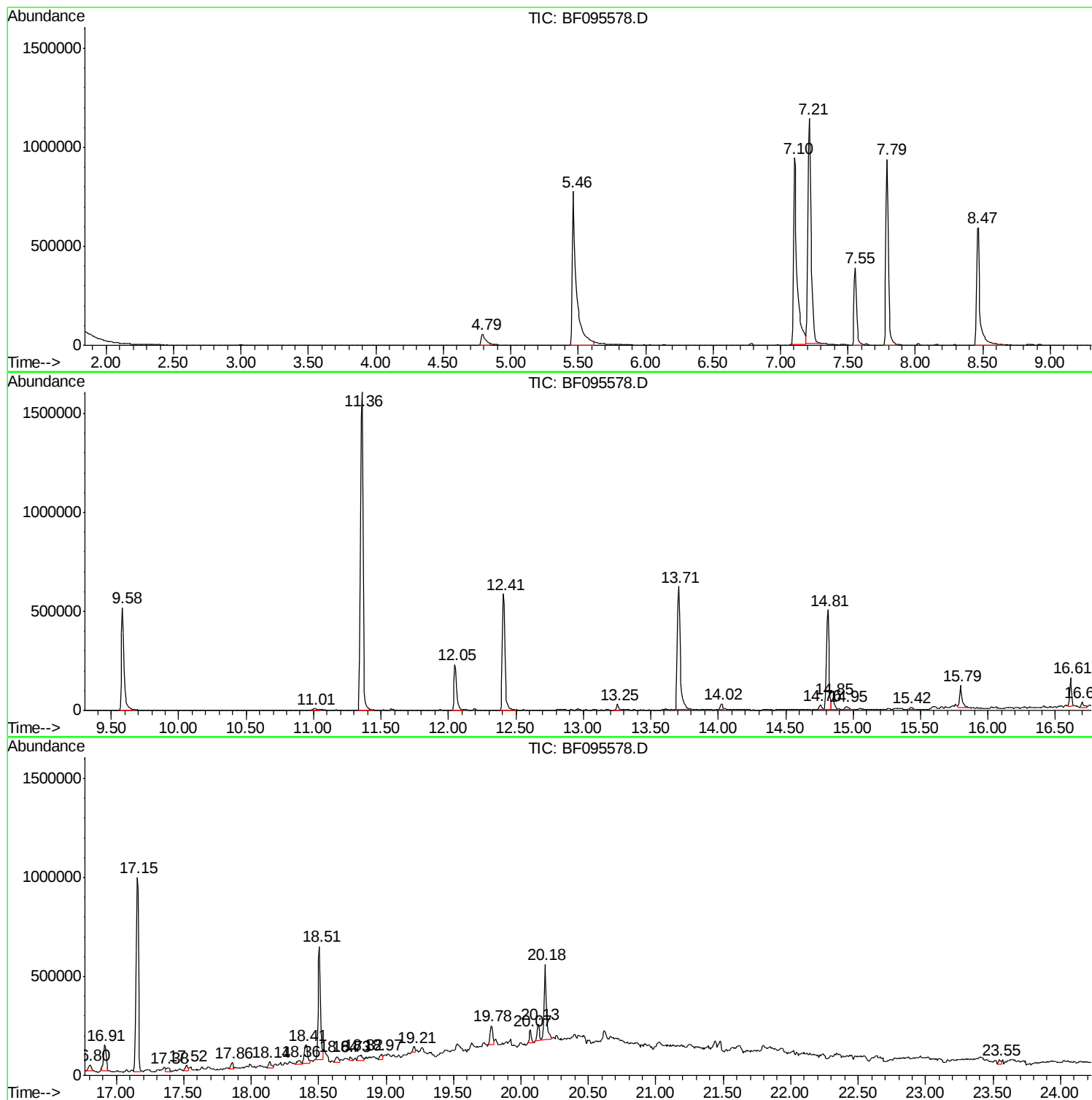
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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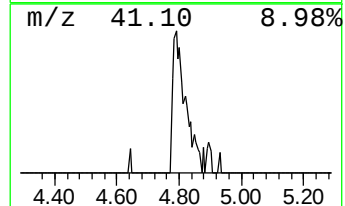
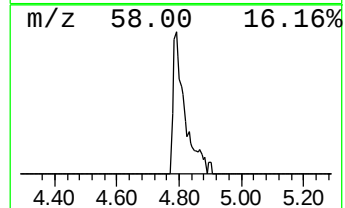
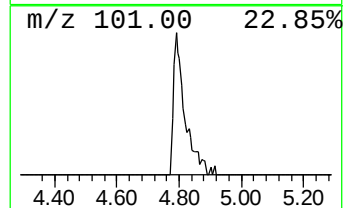
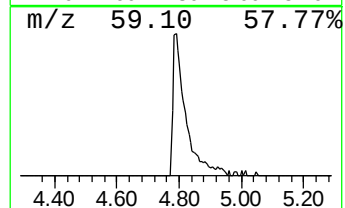
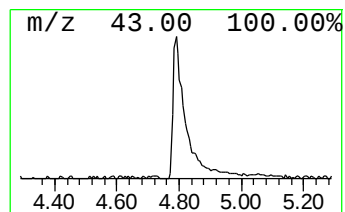
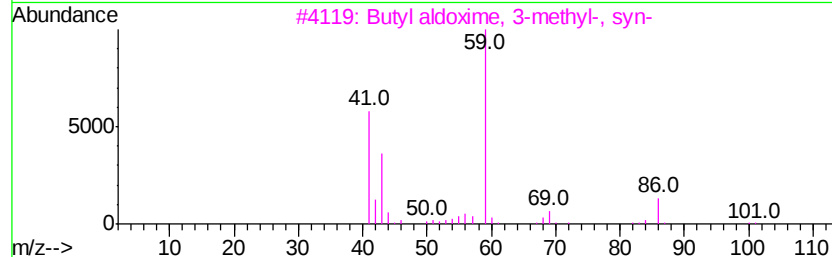
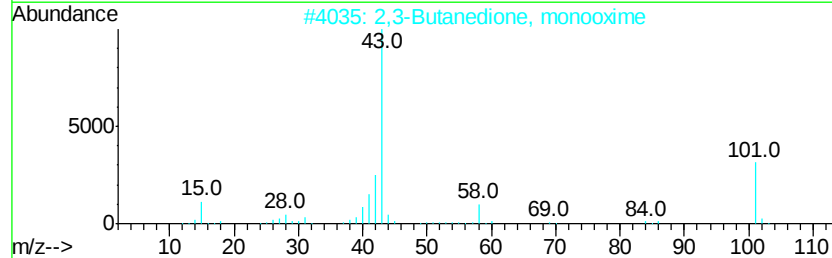
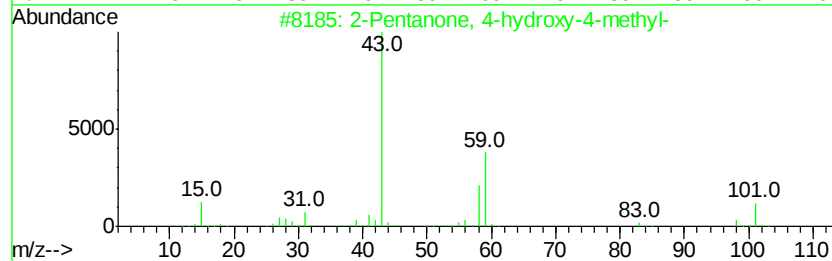
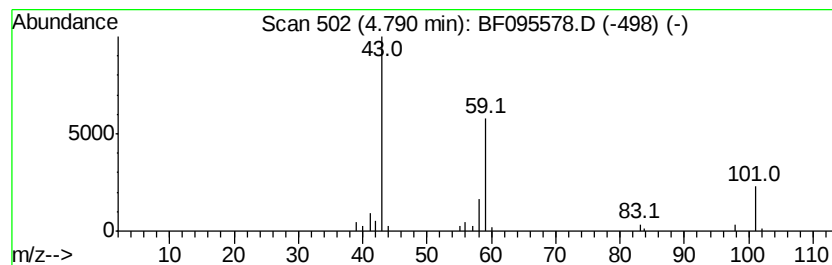
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	5.30 ng	133641	1,4-Dichlorobenzene-d4	7.55

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	12
4			Acetone	58	C3H6O	000067-64-1	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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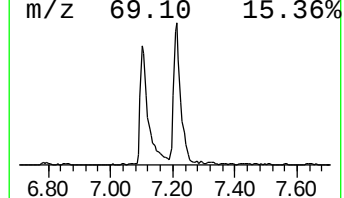
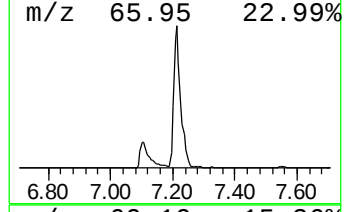
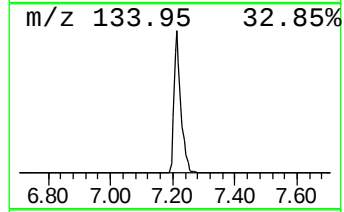
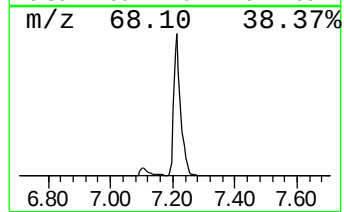
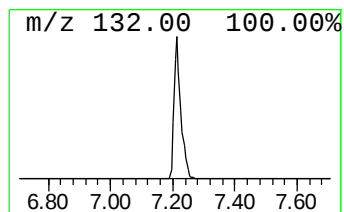
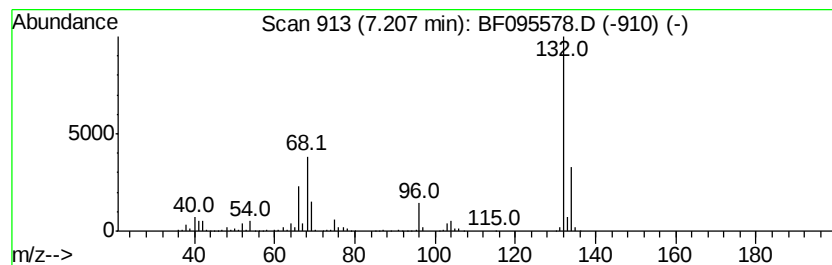
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	71.45 ng	1801070	1,4-Dichlorobenzene-d4	7.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		Xenon	132	Xe	007440-63-3	9



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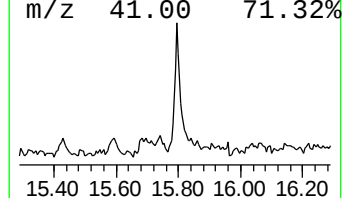
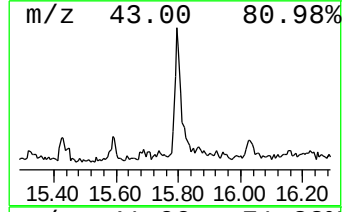
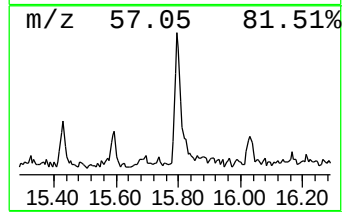
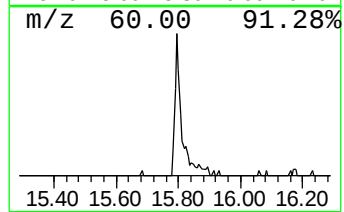
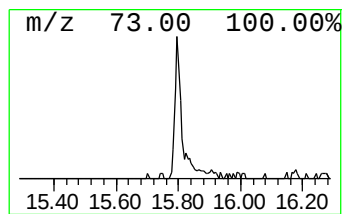
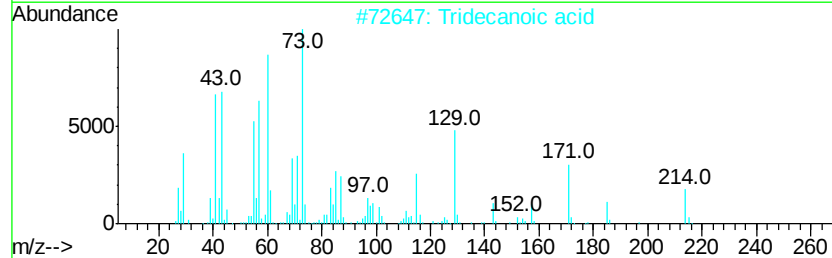
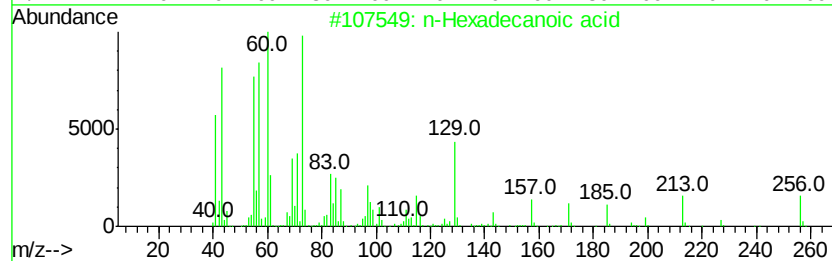
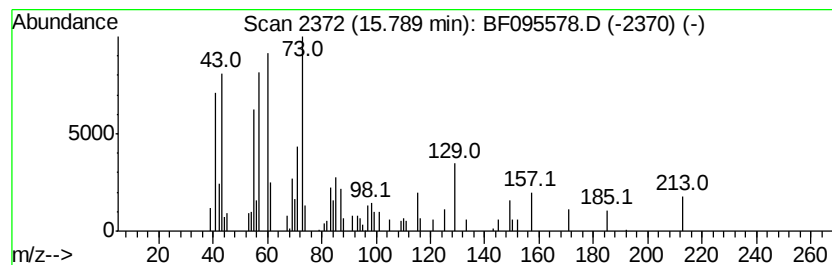
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.79	4.78 ng	155110	Phenanthrene-d10		14.81
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Nonanoic acid	158	C9H18O2	000112-05-0	41



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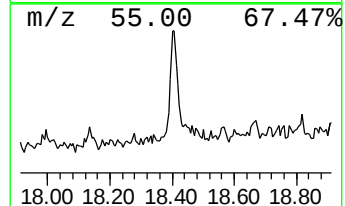
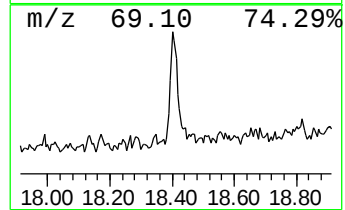
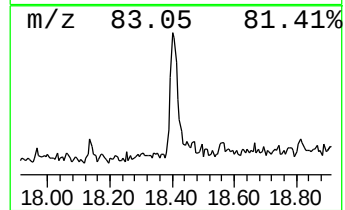
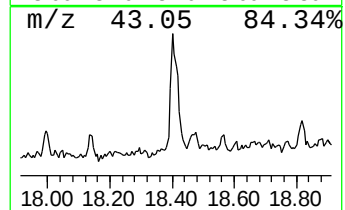
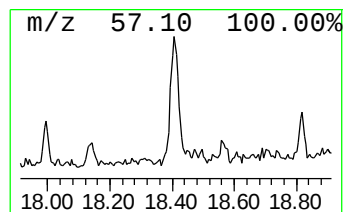
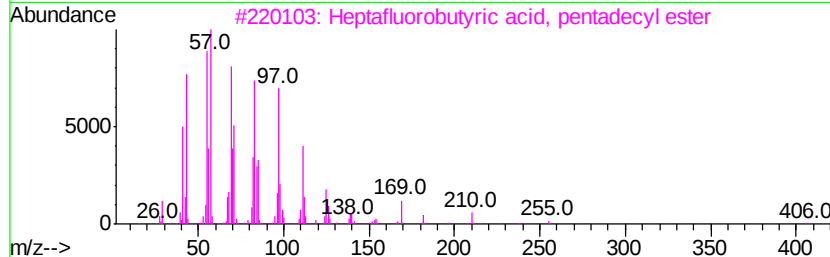
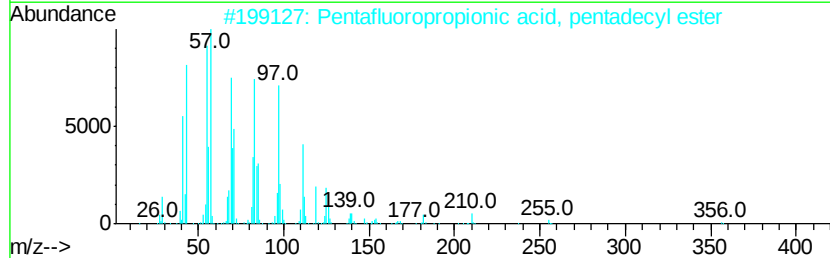
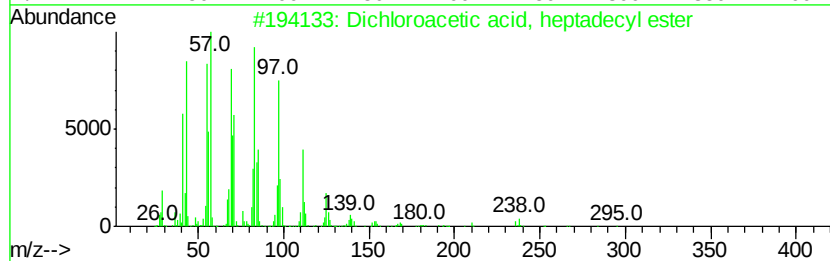
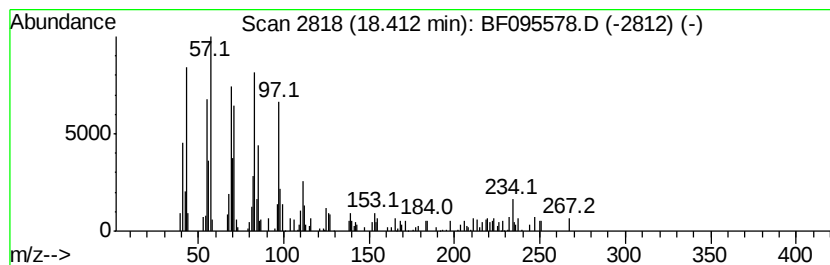
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Dichloroacetic acid, heptadecyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.41	4.69 ng	167266	Chrysene-d12	18.51

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.79	5.3	ng	133641	1	7.55	504143	20.0
unknown7.21	7.21	71.5	ng	1801070	1	7.55	504143	20.0
n-Hexadecanoic acid	15.79	4.8	ng	155110	4	14.81	648980	20.0
Dichloroacetic ac...	18.41	4.7	ng	167266	5	18.51	713169	20.0