

Data Path : Z:\HPCHEM1\BNA N\DATA\BN021918\
 Data File : BN000123.D
 Acq On : 19 Feb 2018 22:47
 Operator : JU/SJ
 Sample : J1577-03
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 COMPOSITE-A-DISSOLVED

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_N\METHODS\8270-BN020718.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	3.234	35	42	51	rBV	454054	922961	2.88%	0.514%
2	3.317	51	56	79	rVB	2953007	4911419	15.33%	2.735%
3	5.934	492	501	513	rBV	4299737	6887516	21.49%	3.836%
4	7.581	771	781	794	rBV	3190784	5254468	16.40%	2.926%
5	7.975	840	848	860	rBV	8169428	13607727	42.46%	7.579%
6	8.458	922	930	942	rBV	2091692	3484735	10.87%	1.941%
7	8.787	978	986	999	rVB	7352167	12288385	38.34%	6.844%
8	9.640	1121	1131	1138	rBV	6041943	10310951	32.17%	5.743%
9	11.299	1403	1413	1424	rBV	3263436	5521250	17.23%	3.075%
10	13.699	1810	1821	1828	rBV	16990321	25129960	78.41%	13.996%
11	14.498	1952	1957	1964	rBV	442641	703770	2.20%	0.392%
12	14.928	2025	2030	2037	rVB	343245	428174	1.34%	0.238%
13	15.069	2047	2054	2062	rVB2	4744479	7372805	23.01%	4.106%
14	15.869	2179	2190	2195	rBV2	392599	726559	2.27%	0.405%
15	16.534	2297	2303	2313	rBV	11568498	16920300	52.80%	9.424%
16	16.722	2330	2335	2344	rBV	305708	487161	1.52%	0.271%
17	17.787	2509	2516	2528	rBV	6109239	8676328	27.07%	4.832%
18	18.628	2653	2659	2669	rBV	880688	1472469	4.59%	0.820%
19	19.875	2866	2871	2879	rBV	471615	703983	2.20%	0.392%
20	20.345	2945	2951	2963	rBV	25009111	32047610	100.00%	17.849%
21	21.563	3154	3158	3175	rBV	1111403	2068936	6.46%	1.152%
22	21.898	3209	3215	3226	rVB	7383108	9627894	30.04%	5.362%
23	24.374	3628	3636	3649	rBV2	4874340	9994538	31.19%	5.566%

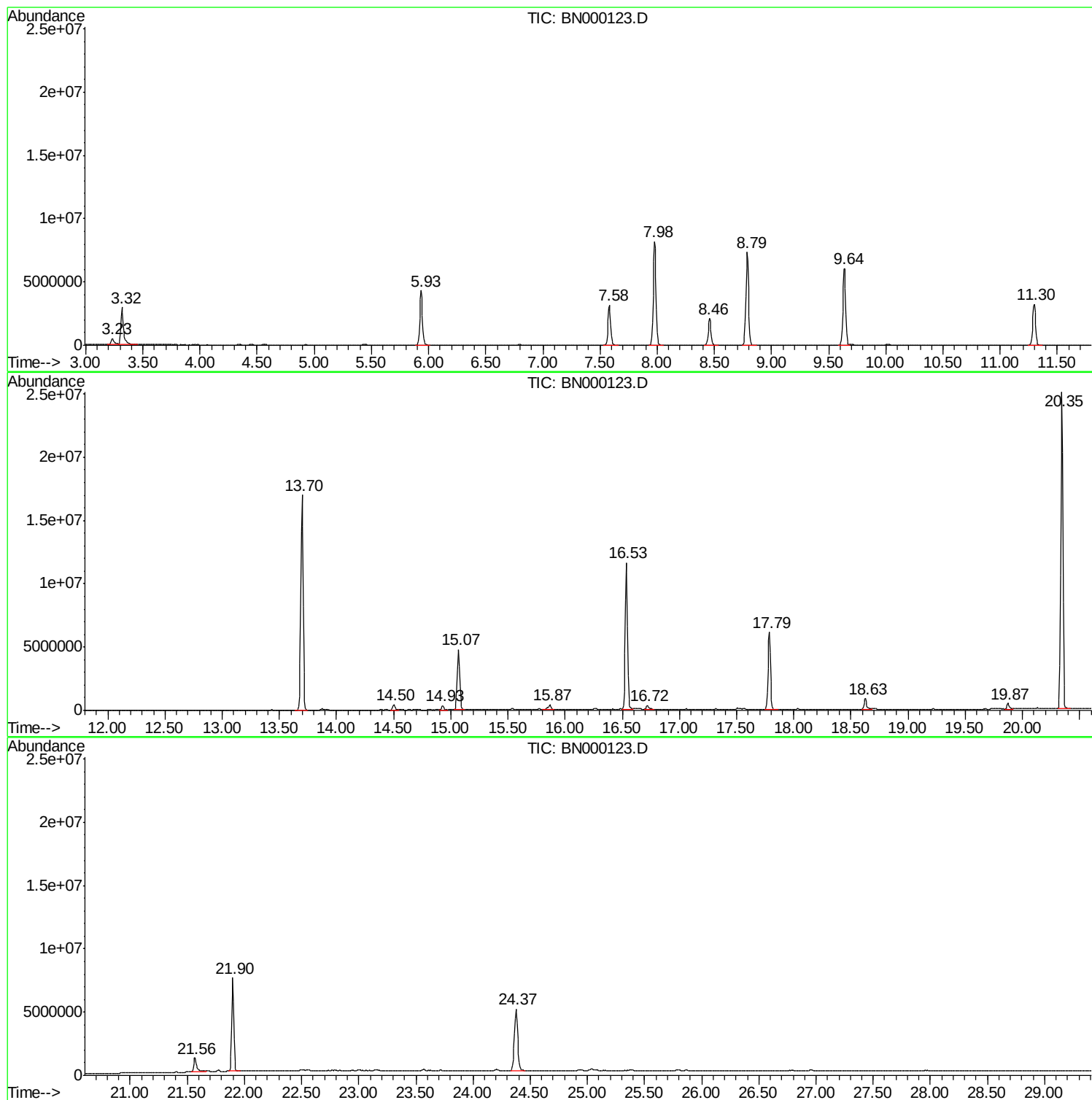
Sum of corrected areas: 179549899

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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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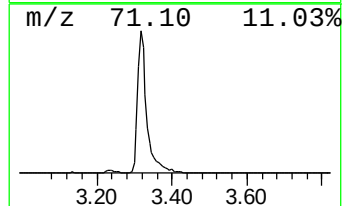
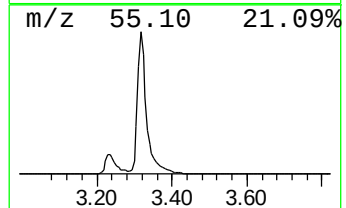
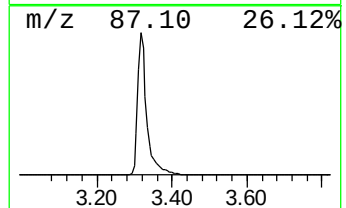
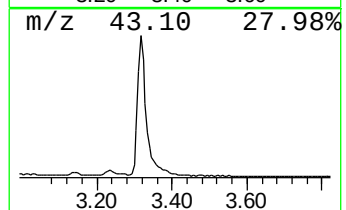
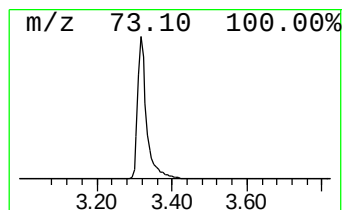
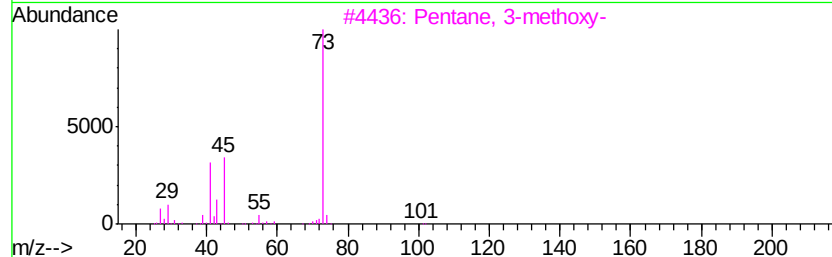
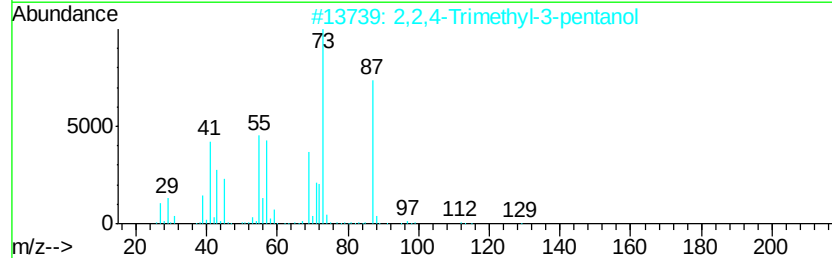
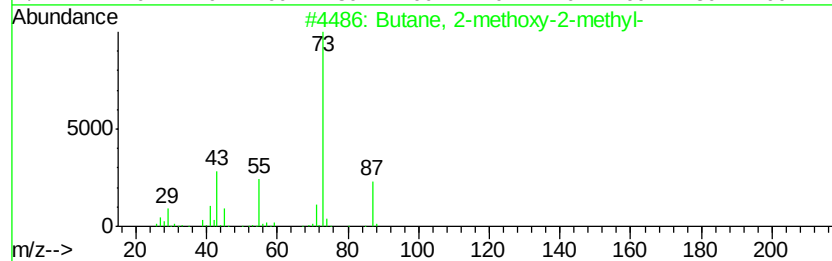
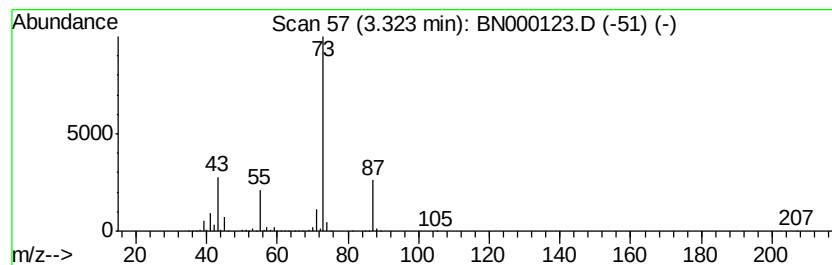
Quant Method : Z:\HPCHEM1\BNA N\METHODS\8270-BN020718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.32	28.19 ng	4911420	1,4-Dichlorobenzene-d4	8.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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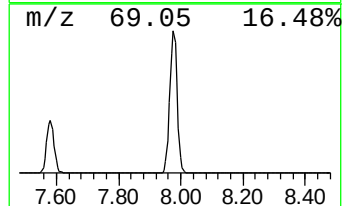
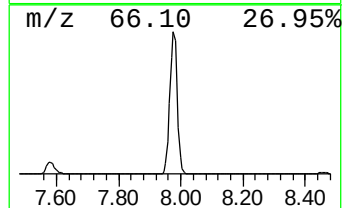
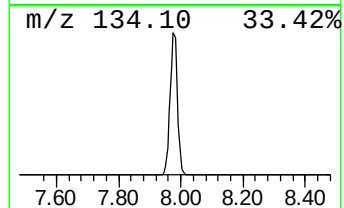
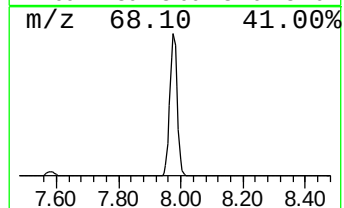
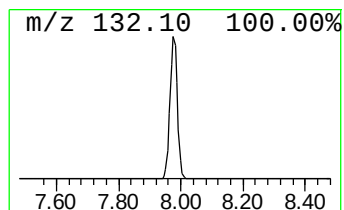
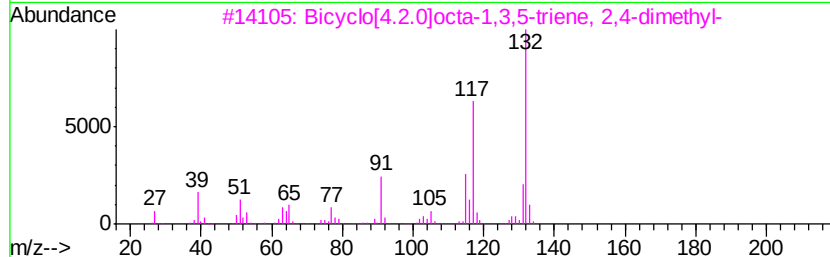
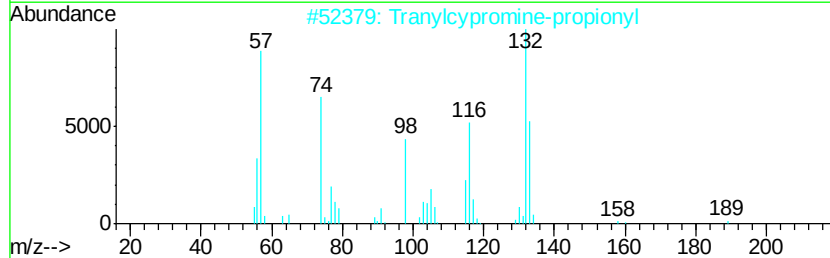
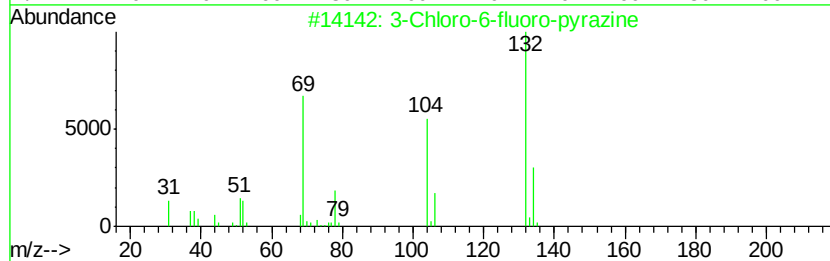
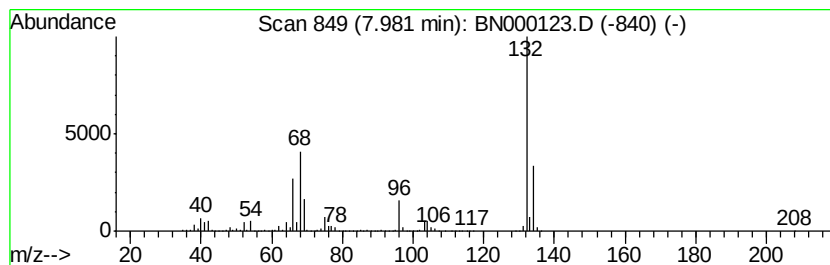
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Peak Number 3 unknown7.98 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.98	78.10 ng	13607700	1,4-Dichlorobenzene-d4	8.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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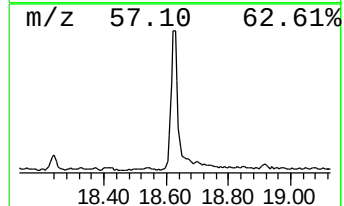
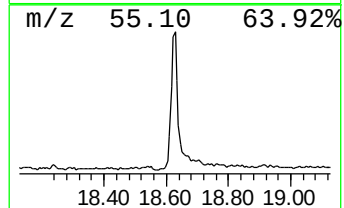
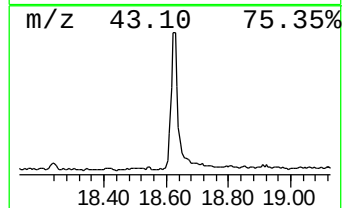
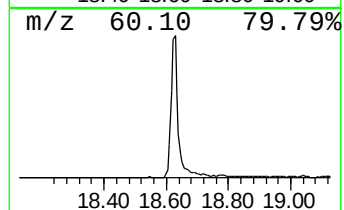
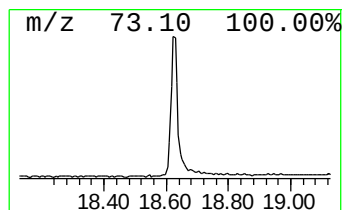
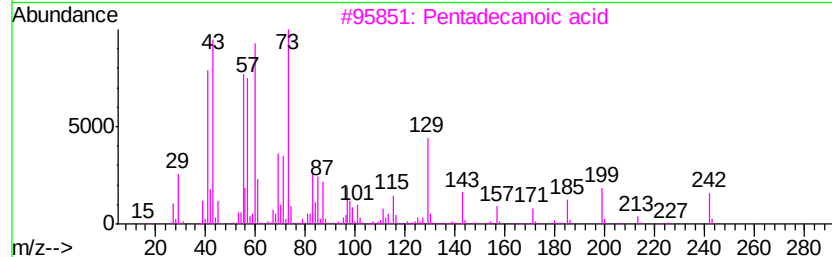
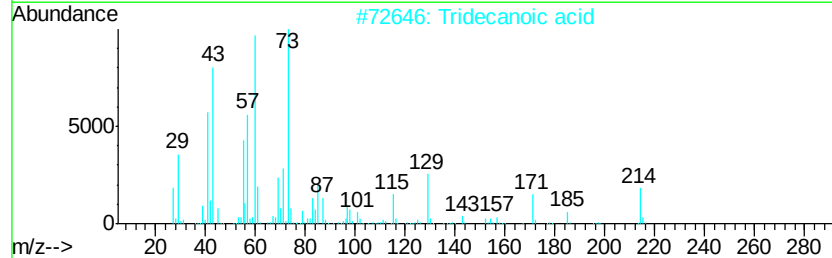
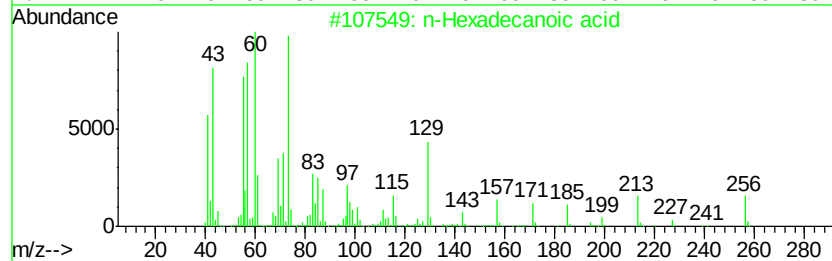
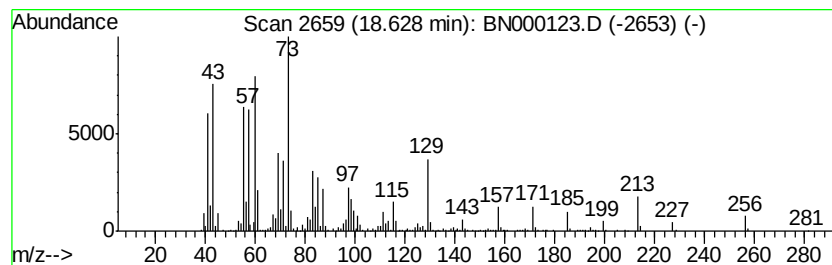
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.63	3.39 ng	1472470	Phenanthrene-d10	17.79	
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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58



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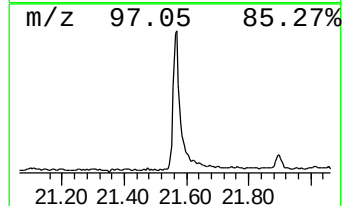
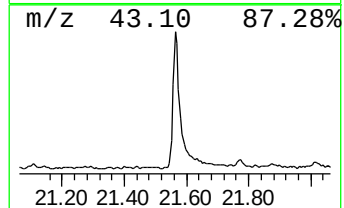
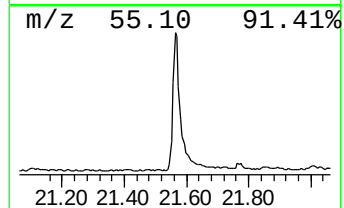
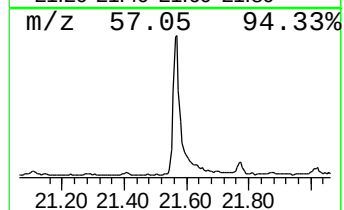
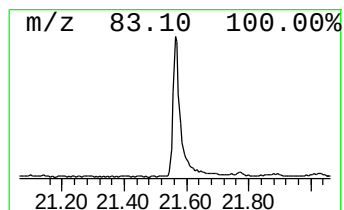
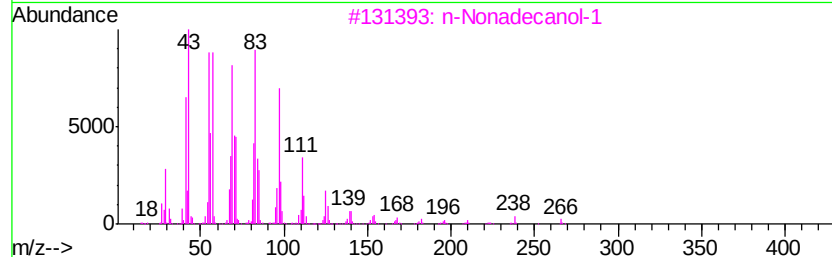
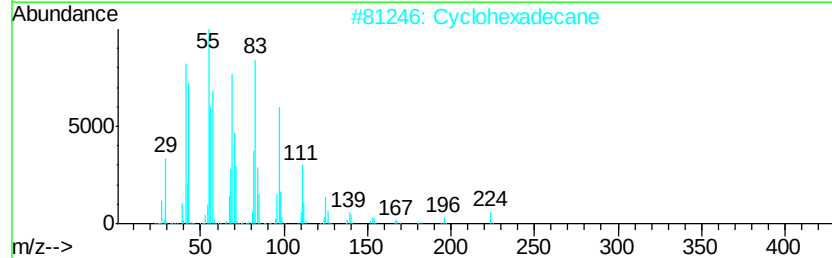
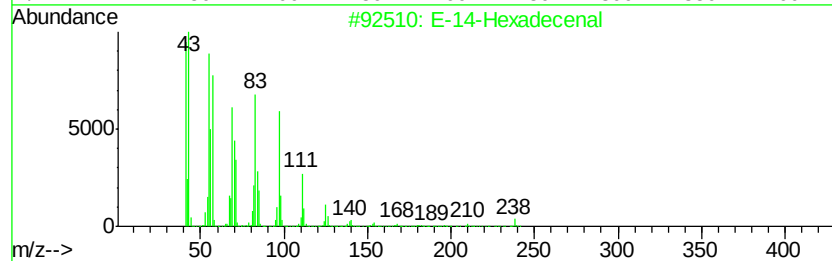
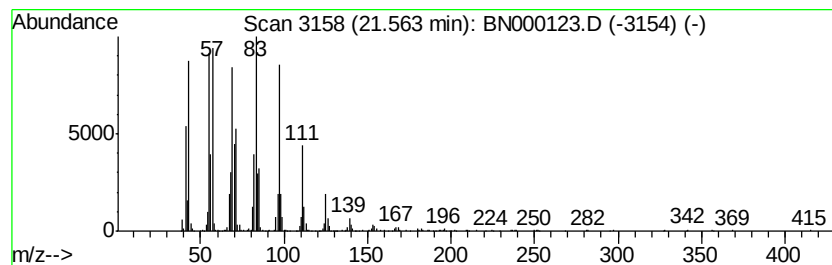
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Peak Number 6 E-14-Hexadecenal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.56	4.30 ng	2068940	Chrysene-d12	21.90	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-14-Hexadecenal	238	C16H30O	330207-53-9	96
2	Cyclohexadecane	224	C16H32	000295-65-8	94
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	1-Heptacosanol	396	C27H56O	002004-39-9	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.32	28.2	ng	4911420	1	8.46	3484740	20.0
unknown7.98	7.98	78.1	ng	13607700	1	8.46	3484740	20.0
n-Hexadecanoic acid	18.63	3.4	ng	1472470	4	17.79	8676330	20.0
E-14-Hexadecenal	21.56	4.3	ng	2068940	5	21.90	9627890	20.0