

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032921\
 Data File : BM029253.D
 Acq On : 29 Mar 2021 20:32
 Operator : CG/JU
 Sample : M1770-21
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MW-102D

Integration Parameters: rteint.p

Integrator: RTE

Smothing : 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:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029253.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.940	5	9	17	rVB6	24972	51059	2.67%	0.313%
2	3.010	17	21	28	rBV	586087	740616	38.76%	4.535%
3	4.898	335	342	350	rVB	17349	34514	1.81%	0.211%
4	5.351	412	419	428	rBV	370263	536201	28.06%	3.284%
5	6.916	678	685	696	rBV	217003	388894	20.35%	2.381%
6	7.751	820	827	835	rVB	436784	685693	35.89%	4.199%
7	8.898	1015	1022	1035	rBV	447055	752176	39.37%	4.606%
8	10.533	1293	1300	1308	rBV	551878	916925	47.99%	5.615%
9	11.463	1451	1458	1465	rBV5	16062	37173	1.95%	0.228%
10	12.998	1713	1719	1729	rBV	1025193	1495549	78.28%	9.158%
11	13.280	1762	1767	1773	rBV6	12055	24283	1.27%	0.149%
12	13.833	1856	1861	1866	rBV2	48033	71133	3.72%	0.436%
13	14.104	1902	1907	1915	rBV5	22378	63107	3.30%	0.386%
14	14.215	1922	1926	1935	rVB	58148	115722	6.06%	0.709%
15	14.374	1947	1953	1961	rBV	758541	1137529	59.54%	6.966%
16	14.798	2021	2025	2032	rVB9	16660	23365	1.22%	0.143%
17	14.945	2040	2050	2053	rBV10	12076	28917	1.51%	0.177%
18	15.557	2149	2154	2162	rBV3	20715	51118	2.68%	0.313%
19	15.857	2199	2205	2214	rBV	731456	1066593	55.83%	6.532%
20	16.157	2253	2256	2261	rVB3	28682	41542	2.17%	0.254%
21	16.521	2310	2318	2322	rBV9	21762	59940	3.14%	0.367%
22	16.892	2377	2381	2385	rBV6	14773	24474	1.28%	0.150%
23	17.115	2412	2419	2425	rBV	880681	1299779	68.03%	7.959%
24	18.015	2566	2572	2590	rBV	470569	816815	42.75%	5.002%
25	18.280	2614	2617	2620	rBV4	23675	32681	1.71%	0.200%
26	18.780	2700	2702	2708	rVB3	26723	29799	1.56%	0.182%
27	19.292	2785	2789	2801	rBV	268004	430182	22.52%	2.634%
28	19.733	2859	2864	2869	rBV	1546388	1910599	100.00%	11.700%
29	21.003	3076	3080	3090	rBV	201355	335389	17.55%	2.054%
30	21.280	3122	3127	3133	rBV	1178639	1521770	79.65%	9.319%
31	23.515	3501	3507	3516	rVB2	862078	1606404	84.08%	9.837%

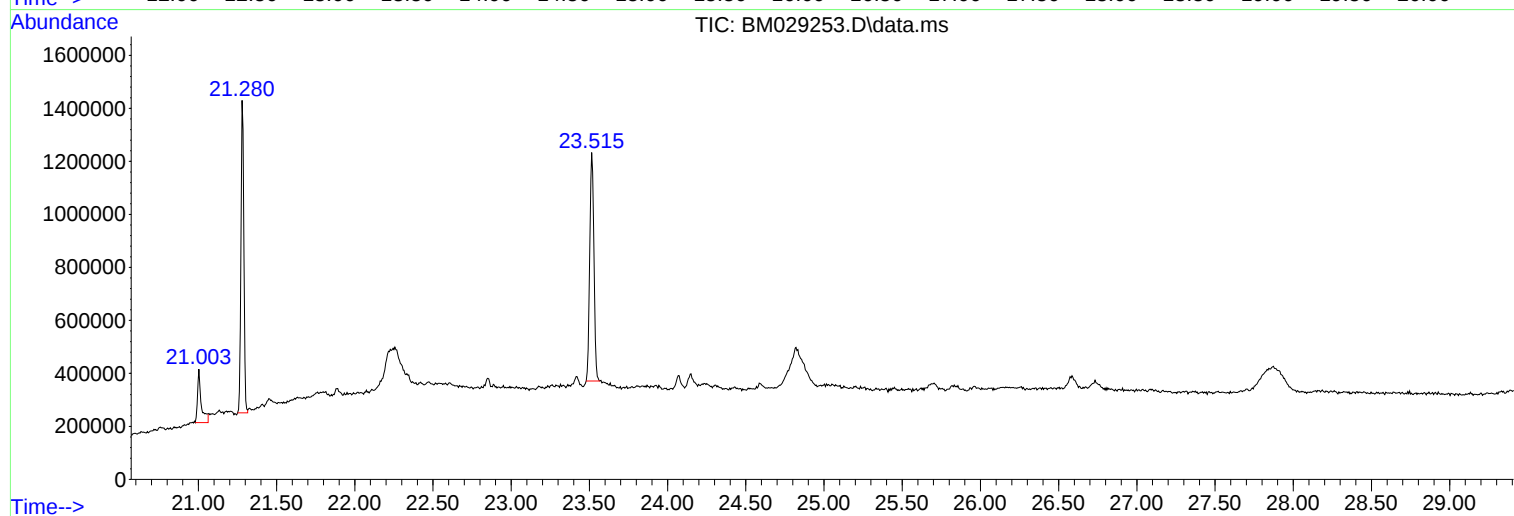
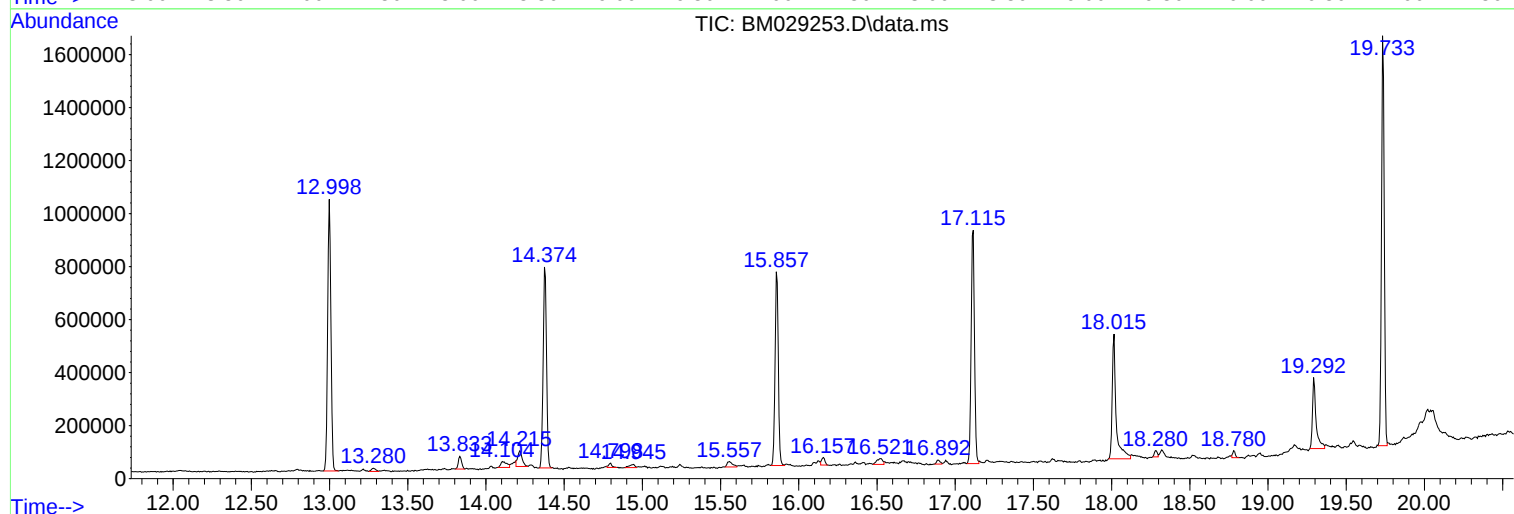
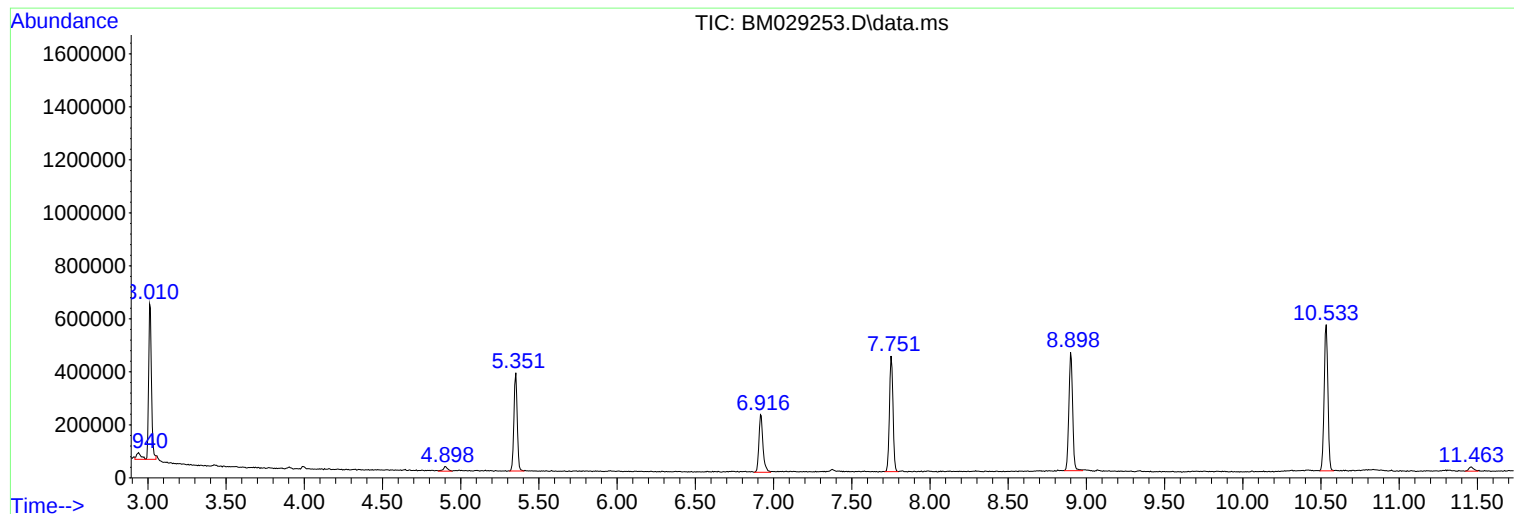
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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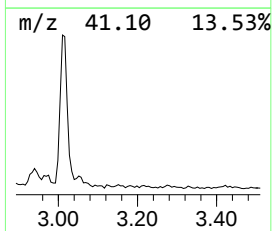
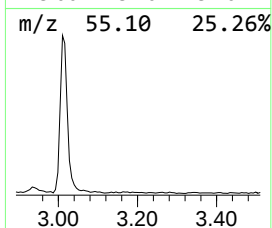
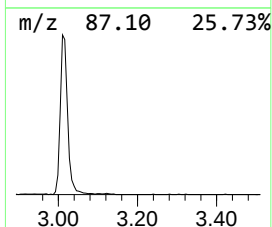
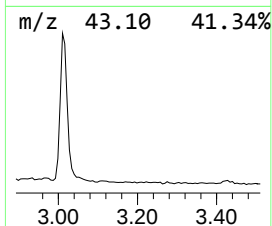
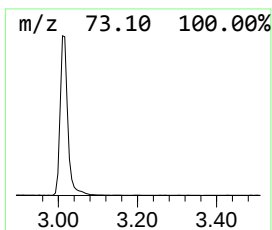
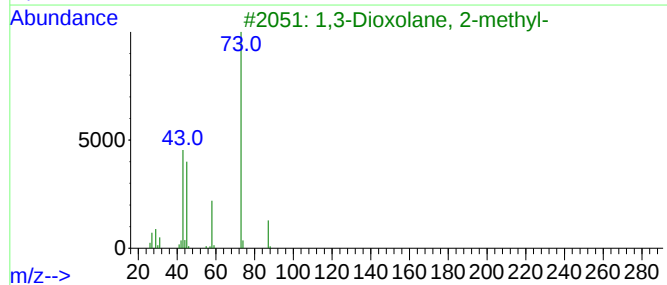
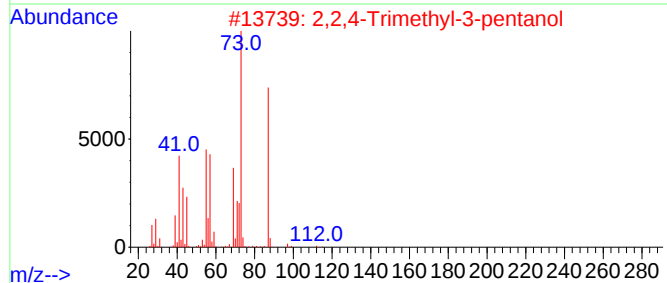
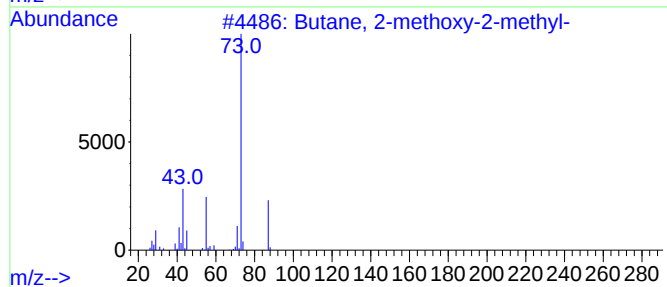
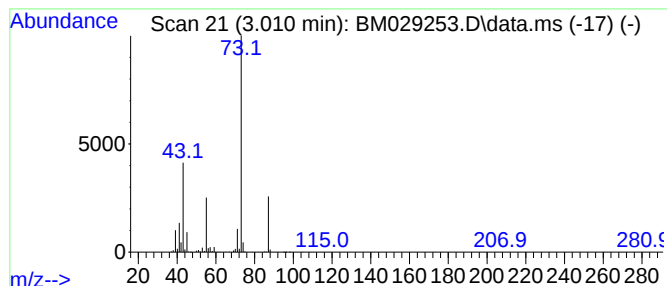
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.010	21.60 ng	740616	1,4-Dichlorobenzene-d4	7.751

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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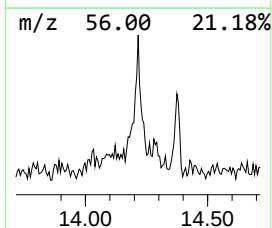
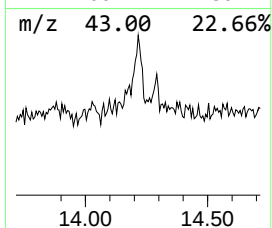
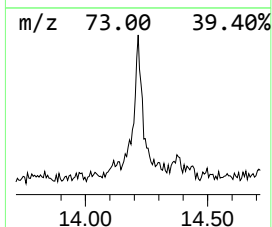
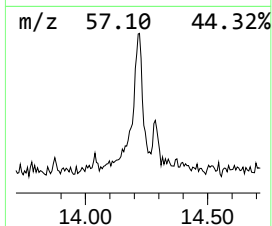
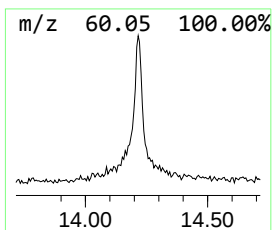
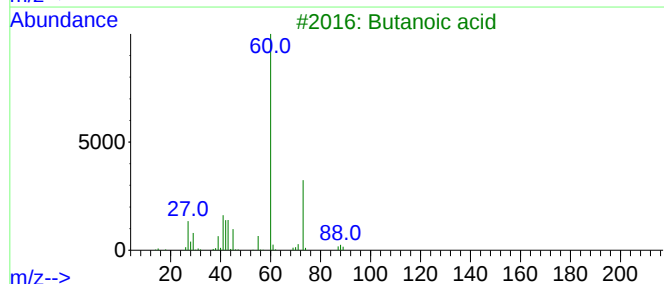
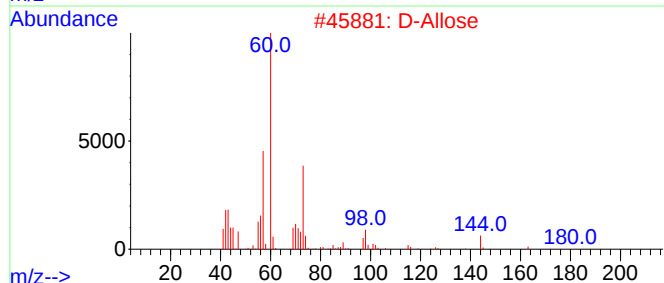
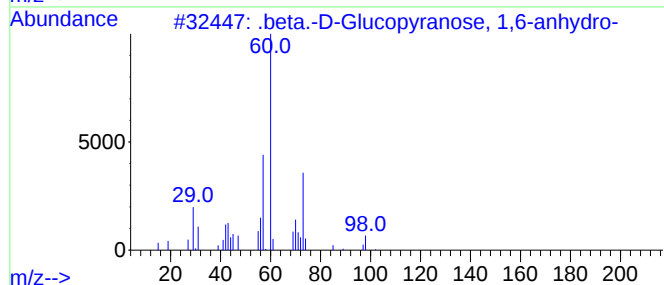
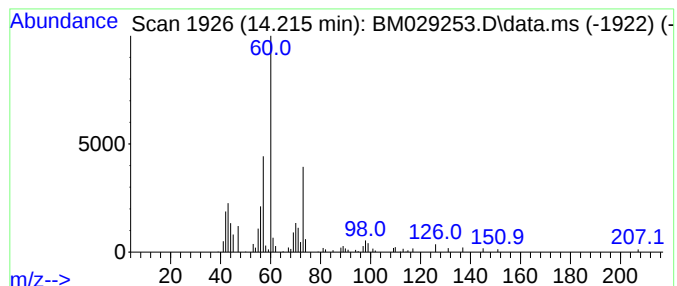
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Peak Number 2 .beta.-D-Glucopyranose, 1,6... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.216	2.03 ng	115722	Acenaphthene-d10	14.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	59
2			D-Allose	180	C6H12O6	002595-97-3	47
3			Butanoic acid	88	C4H8O2	000107-92-6	47
4			Pentanoic acid	102	C5H10O2	000109-52-4	47
5			3,4-Altrosan	162	C6H10O5	1000129-76-4	43



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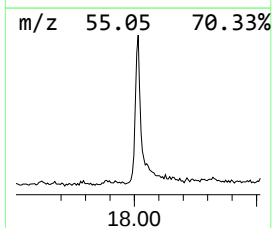
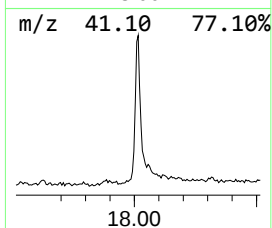
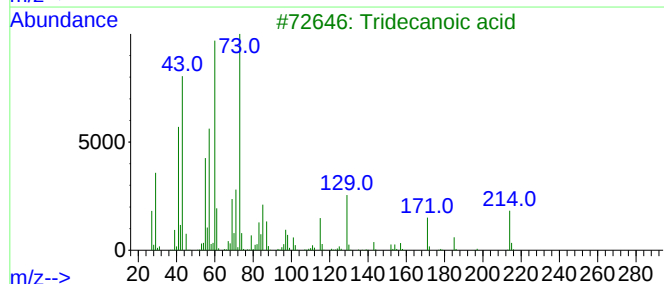
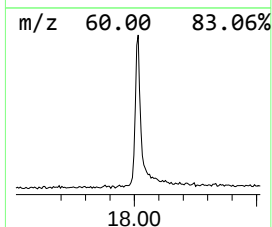
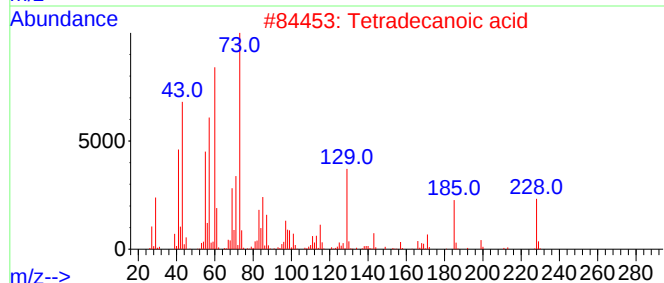
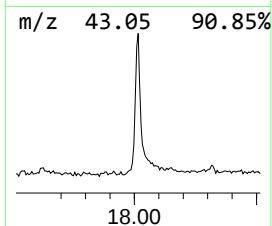
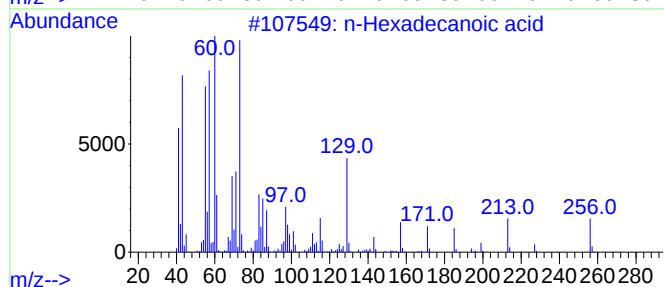
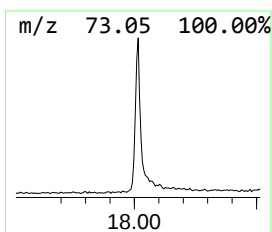
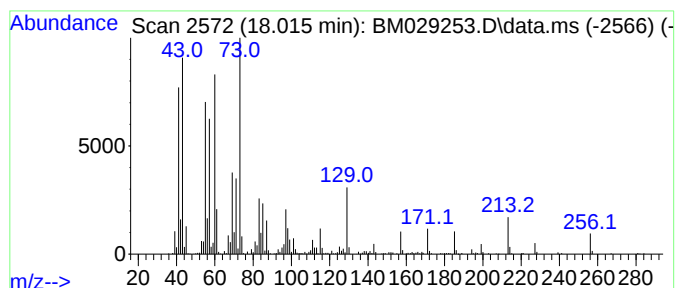
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.015	12.57 ng	816815	Phenanthrene-d10	17.115	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Octadecanoic acid	284	C18H36O2	000057-11-4	60



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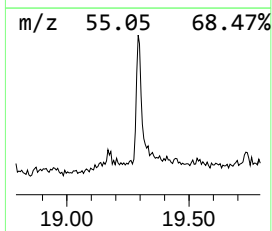
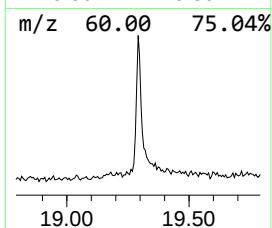
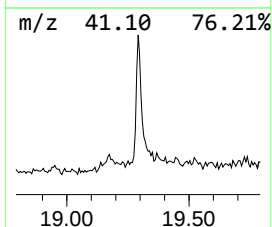
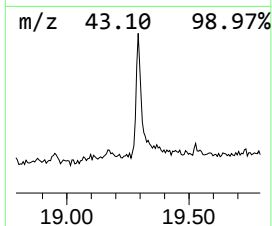
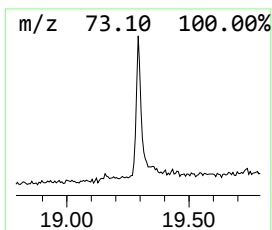
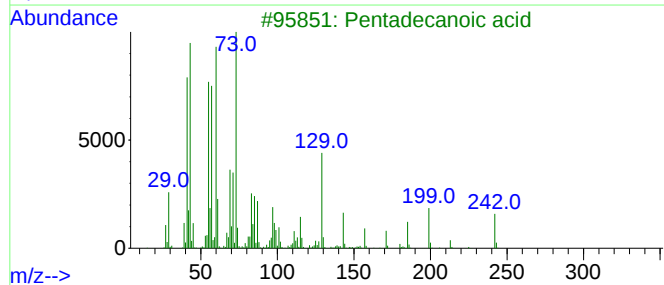
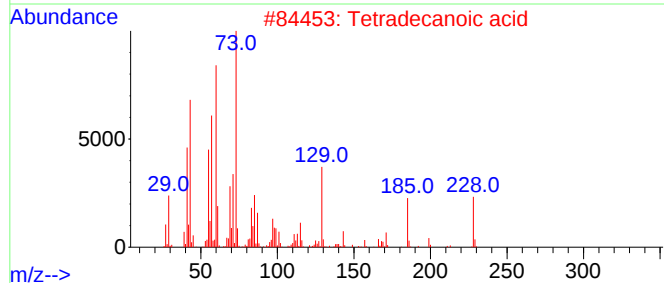
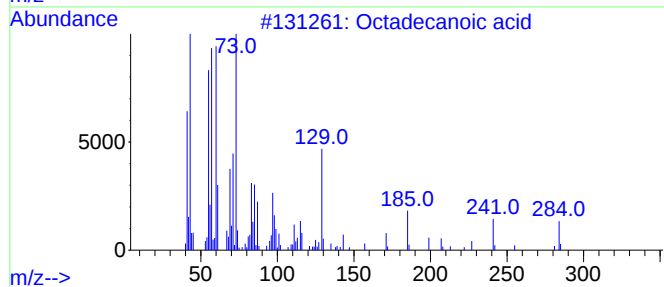
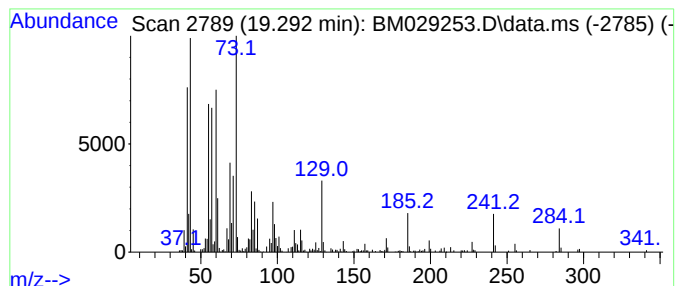
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.292	5.65 ng	430182	Chrysene-d12	21.280

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4			N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	38
5			Oleic Acid	282	C18H34O2	000112-80-1	30



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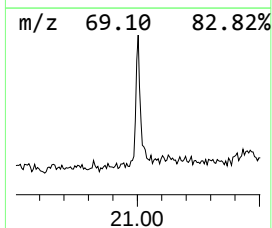
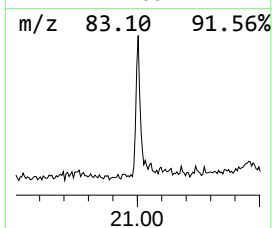
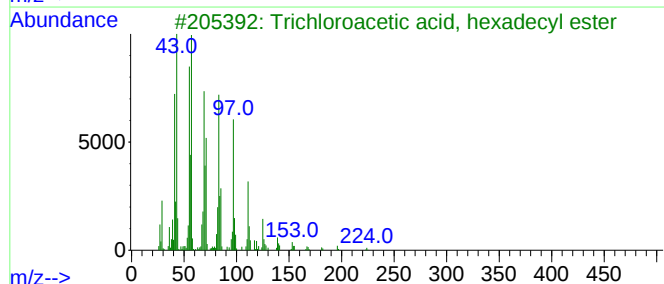
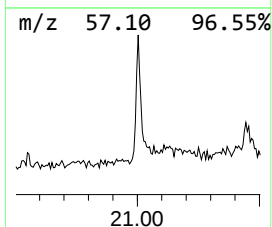
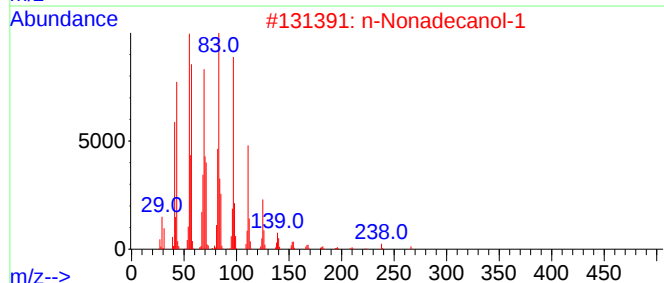
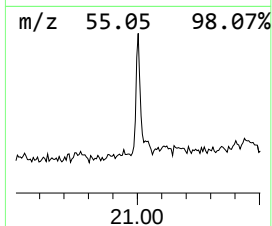
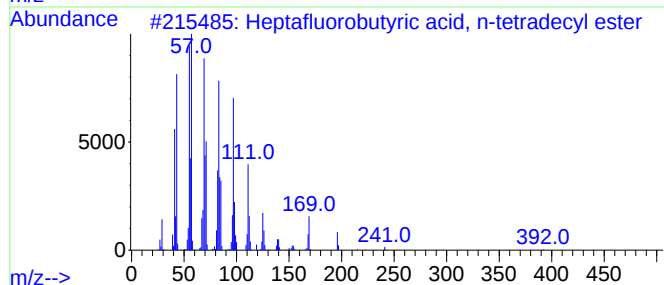
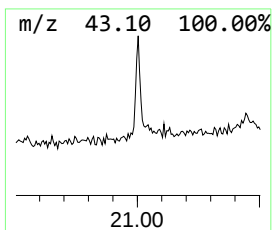
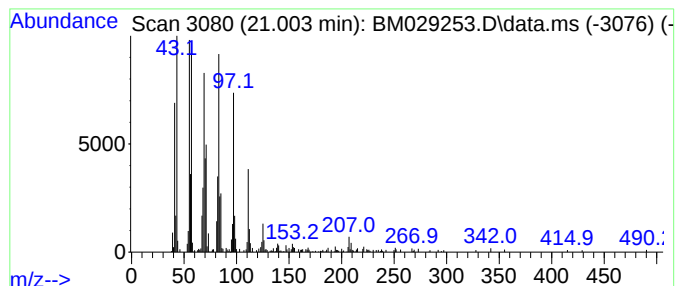
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Peak Number 5 Heptafluorobutyric acid, n-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.003	4.41 ng	335389	Chrysene-d12	21.280

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	91
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4			Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1000164-49-7	91
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.010	21.6	ng	740616	1	7.751	685693	20.0
.beta.-D-Glucop...	14.216	2.0	ng	115722	3	14.374	1137530	20.0
n-Hexadecanoic ...	18.015	12.6	ng	816815	4	17.115	1299780	20.0
Octadecanoic acid	19.292	5.7	ng	430182	5	21.280	1521770	20.0
Heptafluorobuty...	21.003	4.4	ng	335389	5	21.280	1521770	20.0