

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102122\
 Data File : BF130744.D
 Acq On : 21 Oct 2022 14:41
 Operator : CG\JU
 Sample : N5186-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEXAS-SP-1019

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:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102022.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130744.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.740	481	485	504	rVB	305306	489462	18.19%	2.806%
2	5.175	555	559	587	rBV	1765903	2143700	79.65%	12.289%
3	6.222	733	737	763	rBV	2156654	2289815	85.08%	13.127%
4	6.557	791	794	805	rVB	621410	589105	21.89%	3.377%
5	7.134	888	892	910	rBV	1454256	1356419	50.40%	7.776%
6	7.839	1009	1012	1022	rVB	830536	835268	31.03%	4.788%
7	8.263	1081	1084	1093	rVB2	22419	29605	1.10%	0.170%
8	8.439	1110	1114	1116	rBV	36459	35209	1.31%	0.202%
9	8.863	1183	1186	1189	rVB	38153	28445	1.06%	0.163%
10	8.922	1191	1196	1199	rBV	2793870	2691455	100.00%	15.429%
11	8.998	1205	1209	1214	rVB	88355	76161	2.83%	0.437%
12	9.316	1259	1263	1265	rVB	38699	35052	1.30%	0.201%
13	9.527	1295	1299	1302	rBV	71794	57676	2.14%	0.331%
14	9.586	1306	1309	1322	rVB	1101637	942649	35.02%	5.404%
15	10.022	1380	1383	1386	rVB	48065	36851	1.37%	0.211%
16	10.380	1440	1444	1460	rVB	1831621	1683742	62.56%	9.652%
17	11.069	1558	1561	1569	rBV	900104	732445	27.21%	4.199%
18	11.139	1569	1573	1578	rVB2	44286	38240	1.42%	0.219%
19	11.610	1644	1653	1664	rBV2	108917	177523	6.60%	1.018%
20	12.286	1764	1768	1780	rBV2	27516	72990	2.71%	0.418%
21	12.386	1780	1785	1793	rBV2	58271	91699	3.41%	0.526%
22	12.510	1804	1806	1811	rVB2	20733	28874	1.07%	0.166%
23	12.651	1826	1830	1833	rBV	2350535	1974593	73.37%	11.320%
24	13.704	2005	2009	2023	rBV	460468	532185	19.77%	3.051%
25	15.074	2239	2242	2254	rVB	344600	416726	15.48%	2.389%
26	17.639	2670	2678	2686	rBV6	18541	58102	2.16%	0.333%

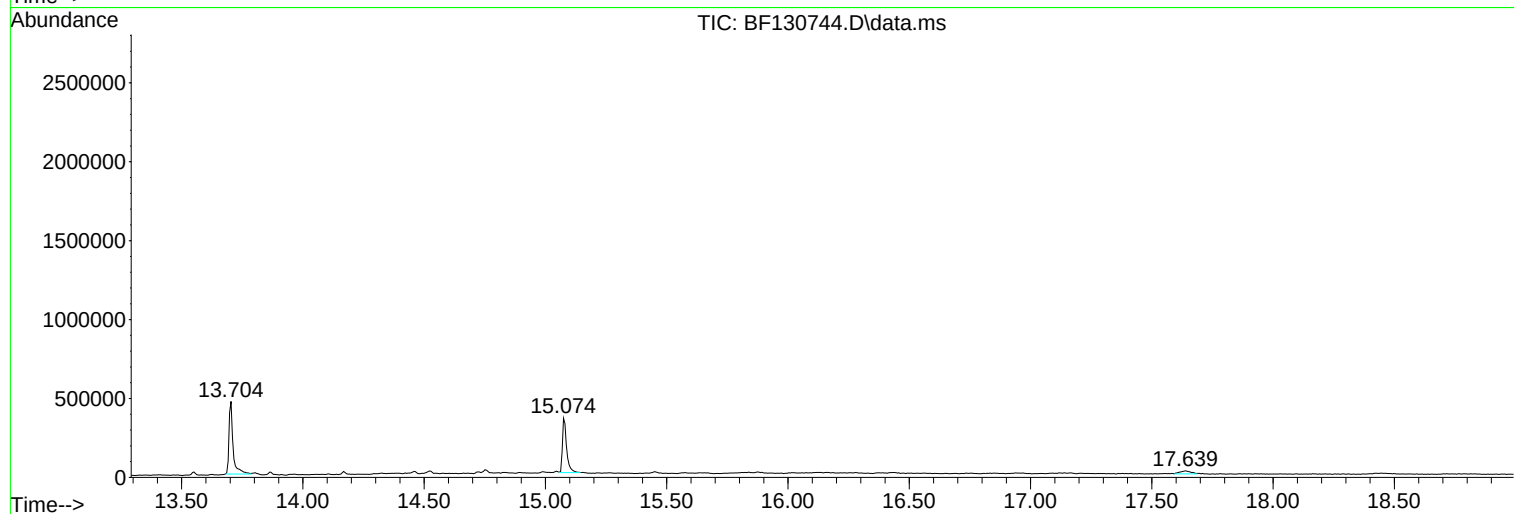
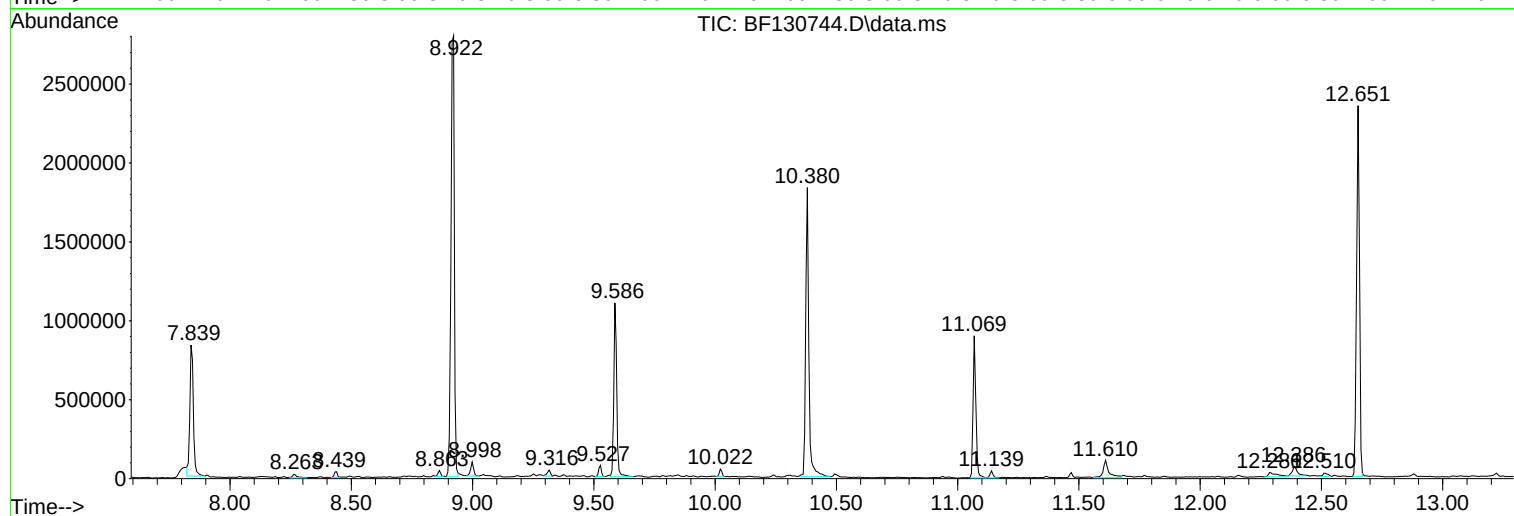
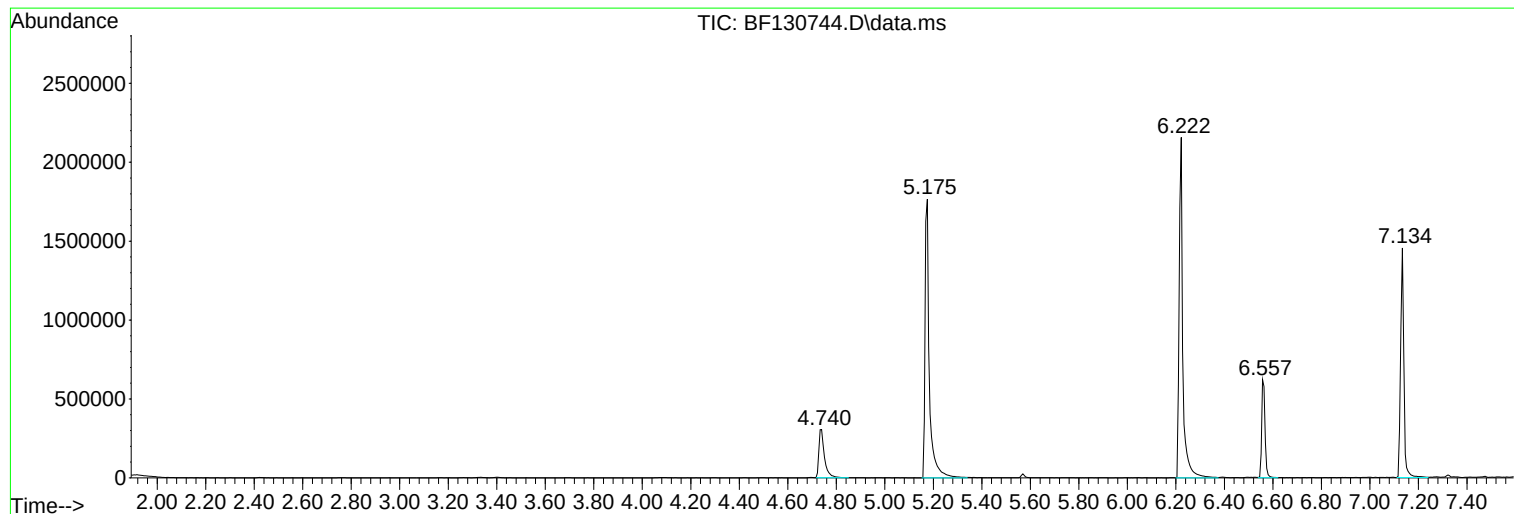
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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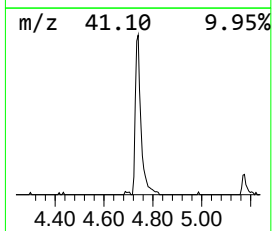
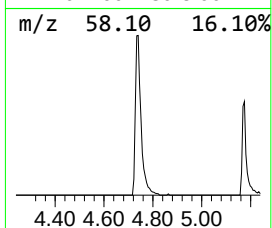
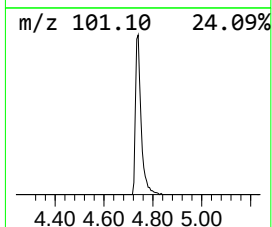
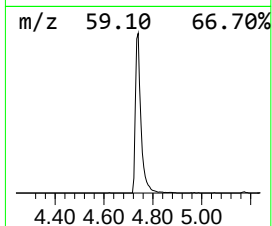
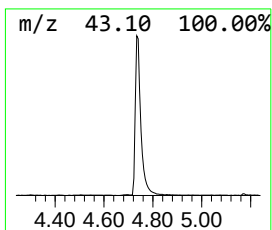
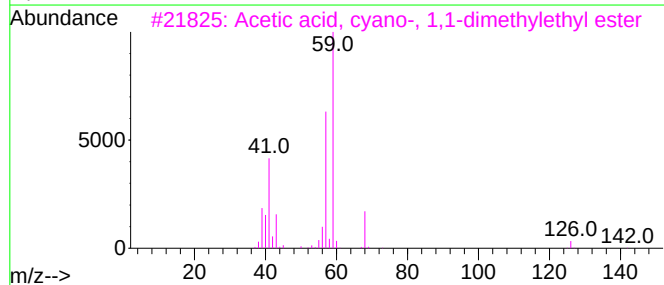
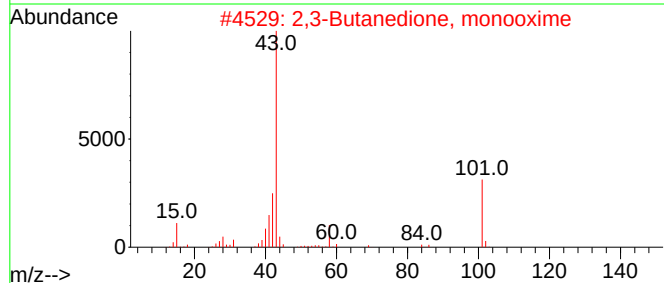
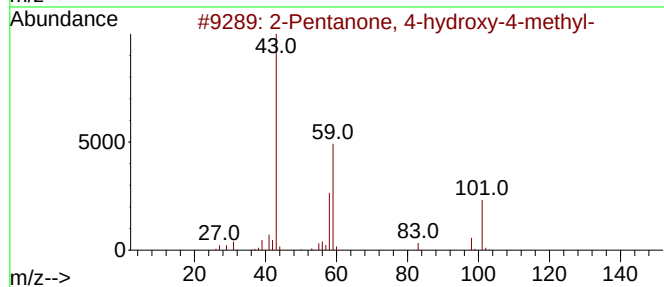
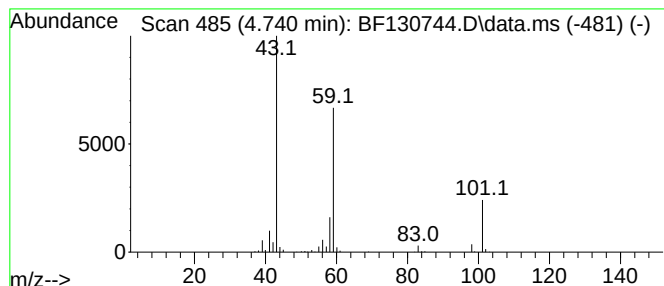
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.740	16.62 ng	489462	1,4-Dichlorobenzene-d4	6.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



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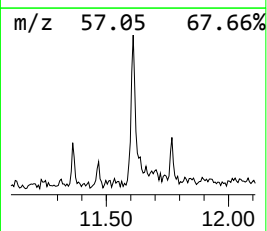
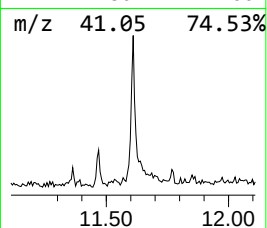
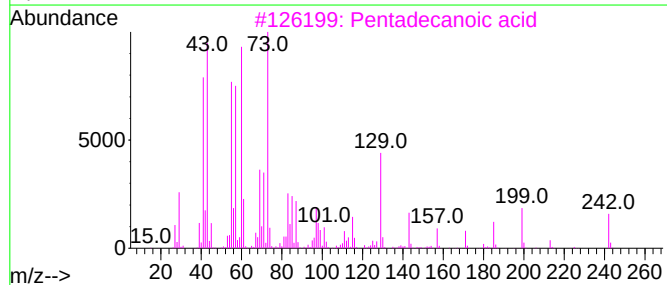
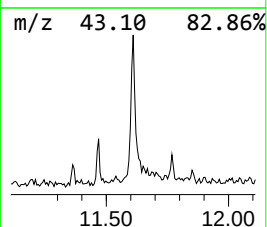
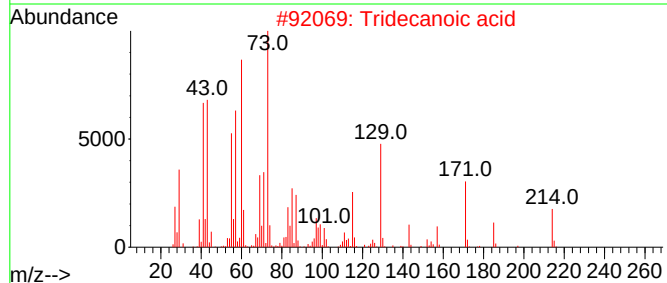
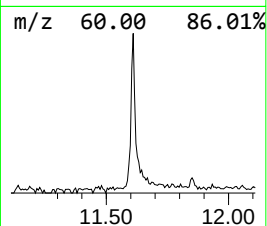
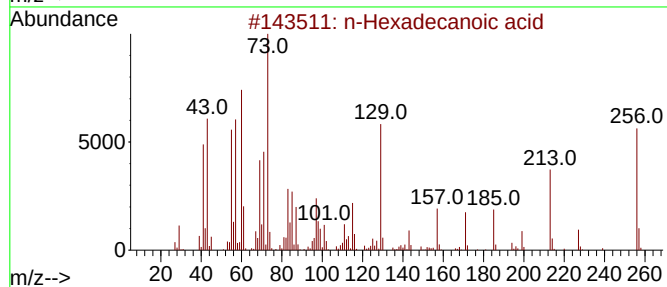
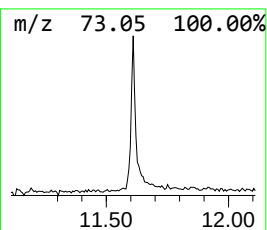
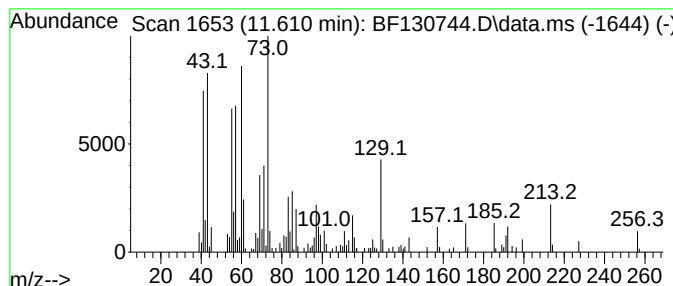
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.610	4.85 ng	177523	Phenanthrene-d10		11.069	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	80
5	n-Decanoic acid		172	C10H20O2	000334-48-5	76



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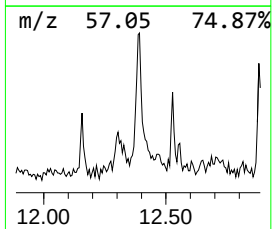
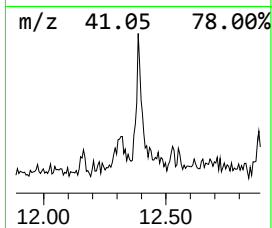
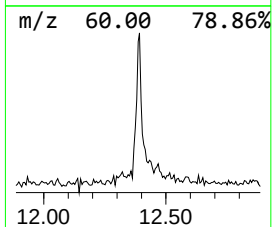
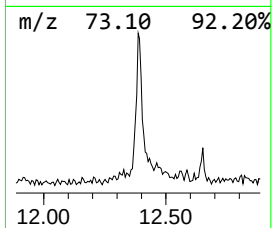
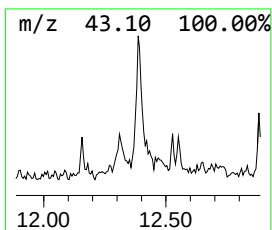
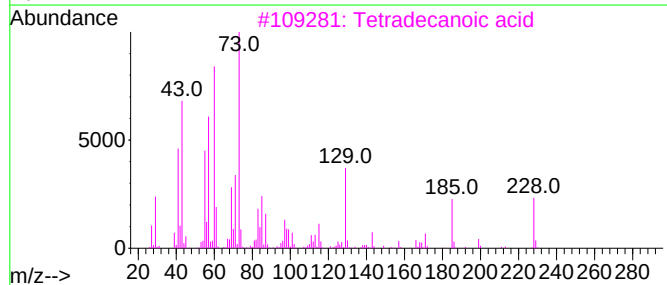
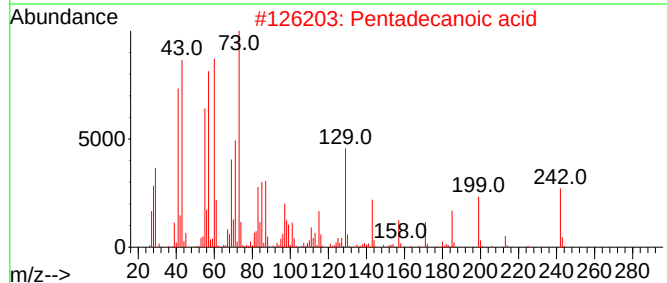
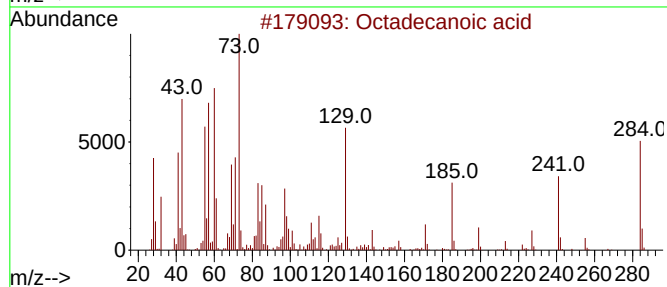
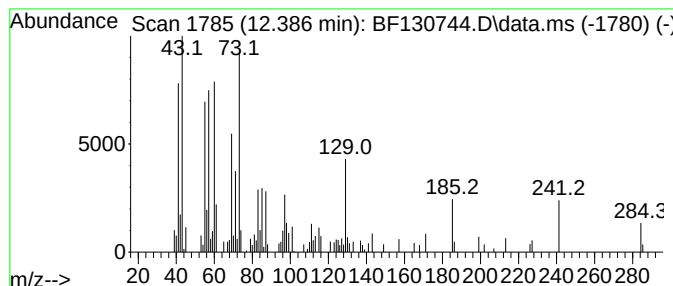
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Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.386	3.45 ng	91699	Chrysene-d12	13.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			Undecanoic acid	186	C11H22O2	000112-37-8	55



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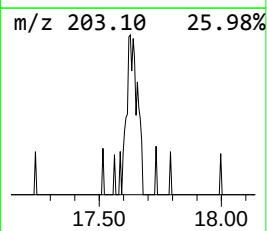
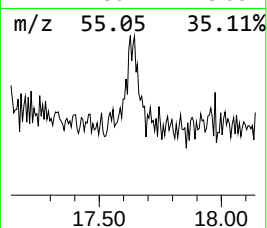
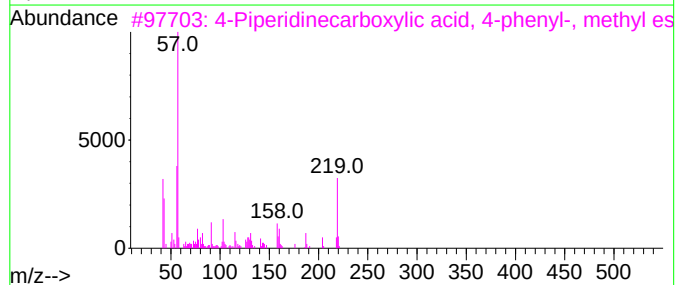
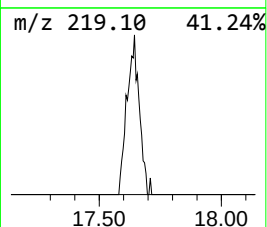
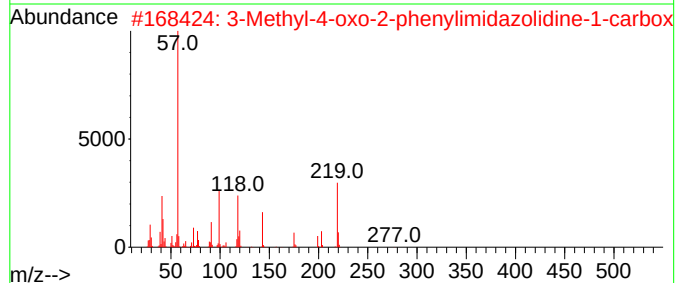
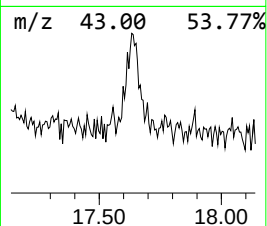
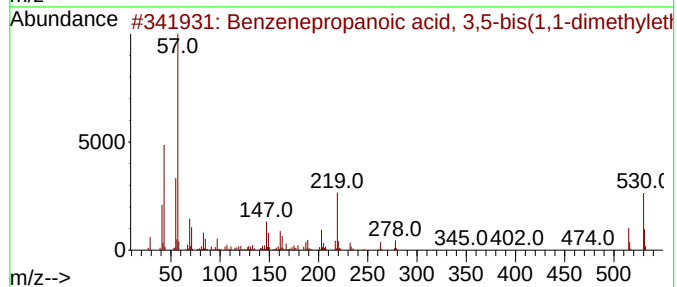
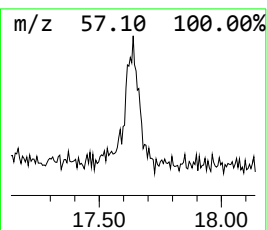
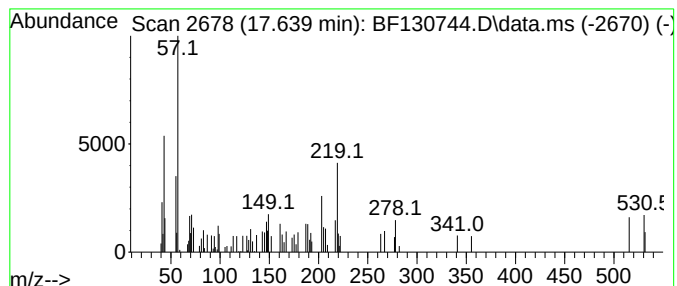
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Peak Number 4 Benzenepropanoic acid, 3,5-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.639	2.79 ng	58102	Perylene-d12	15.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenepropanoic acid, 3,5-bis(1...	530	C35H62O3	002082-79-3	78
2			3-Methyl-4-oxo-2-phenylimidazoli...	276	C15H20N2O3	1000191-10-7	10
3			4-Piperidinecarboxylic acid, 4-p...	219	C13H17NO2	054824-07-6	10
4			Propanamide, N-ethyl-N-(3-methyl...	219	C14H21NO	1000308-12-5	9
5			2,4,5-Trimethylaniline, N-trimet...	219	C14H21NO	1000461-90-2	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.740	16.6	ng	489462	1	6.563	589105	20.0
n-Hexadecanoic ...	11.610	4.8	ng	177523	4	11.069	732445	20.0
Octadecanoic acid	12.386	3.5	ng	91699	5	13.704	532185	20.0
Benzenepropanoi...	17.639	2.8	ng	58102	6	15.074	416726	20.0