

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP012423\
 Data File : BP013589.D
 Acq On : 25 Jan 2023 01:35
 Operator : CG/JU
 Sample : 01260-13
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TP-25

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_P\Methods\8270E-BP012323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP013589.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.222	3	6	22	rVB	2759635	3395856	20.35%	3.532%
2	5.216	339	345	354	rBV	2466172	3447666	20.66%	3.586%
3	5.687	418	425	435	rBV	5955804	8850678	53.03%	9.206%
4	7.305	691	700	709	rBV	5505237	9215989	55.22%	9.586%
5	8.157	837	845	852	rBV	1455543	2297456	13.77%	2.390%
6	9.328	1036	1044	1052	rBV	3333230	5689665	34.09%	5.918%
7	10.987	1315	1326	1333	rBV	1957969	3322533	19.91%	3.456%
8	13.422	1732	1740	1754	rBV	8406412	12862049	77.06%	13.379%
9	13.610	1764	1772	1780	rVB2	94588	167772	1.01%	0.175%
10	14.792	1962	1973	1984	rBV	2902605	4286645	25.68%	4.459%
11	16.145	2198	2203	2209	rVB	255917	349316	2.09%	0.363%
12	16.275	2218	2225	2248	rBV	6291832	9743719	58.38%	10.135%
13	16.516	2258	2266	2272	rVB3	90283	173064	1.04%	0.180%
14	17.545	2434	2441	2446	rBV	3410477	4972180	29.79%	5.172%
15	18.398	2581	2586	2591	rBV	427147	568373	3.41%	0.591%
16	19.622	2790	2794	2799	rBV	141221	191544	1.15%	0.199%
17	19.880	2835	2838	2847	rVB	163633	255694	1.53%	0.266%
18	20.074	2865	2871	2876	rBV	13619214	16690455	100.00%	17.361%
19	21.292	3074	3078	3088	rBV	1095848	1346262	8.07%	1.400%
20	21.504	3111	3114	3120	rVB	149424	187744	1.12%	0.195%
21	21.616	3127	3133	3138	rBV	2940076	4192188	25.12%	4.361%
22	21.657	3138	3140	3145	rVB	209350	254566	1.53%	0.265%
23	24.204	3565	3573	3583	rVB2	1664568	3674913	22.02%	3.823%

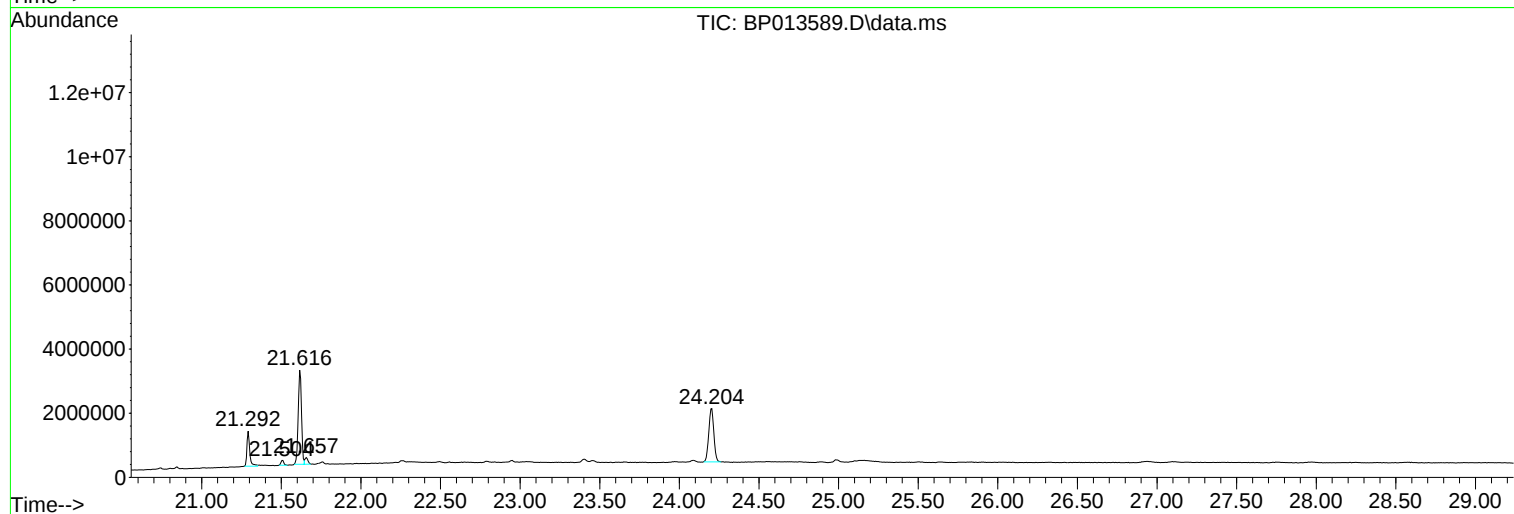
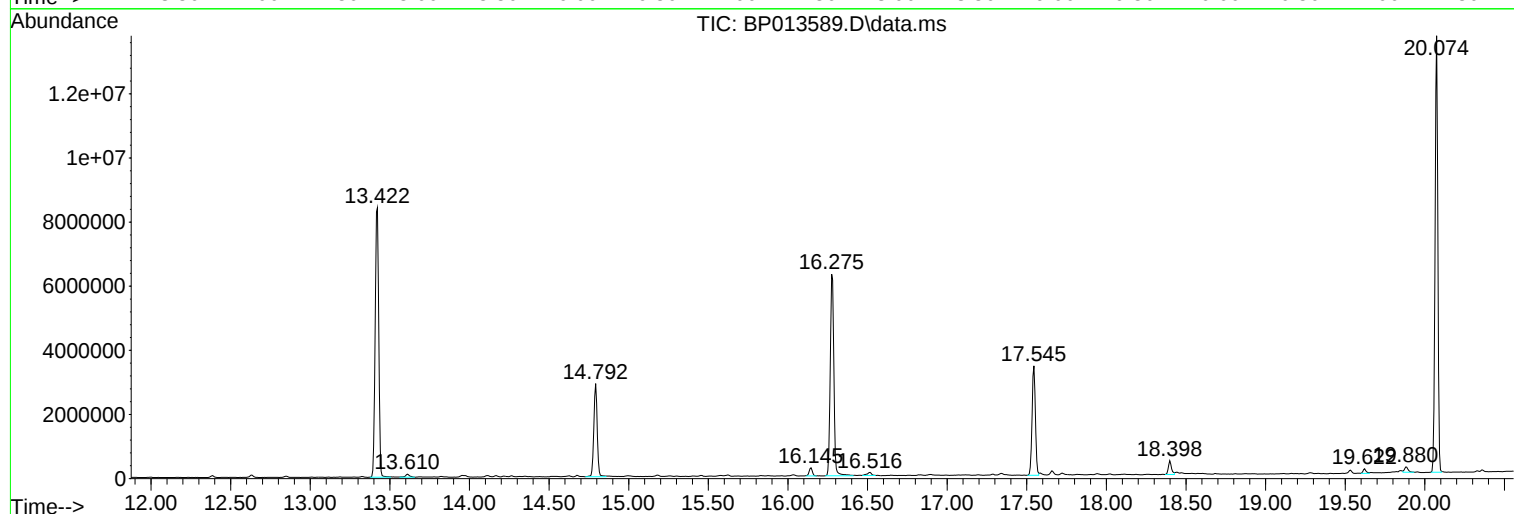
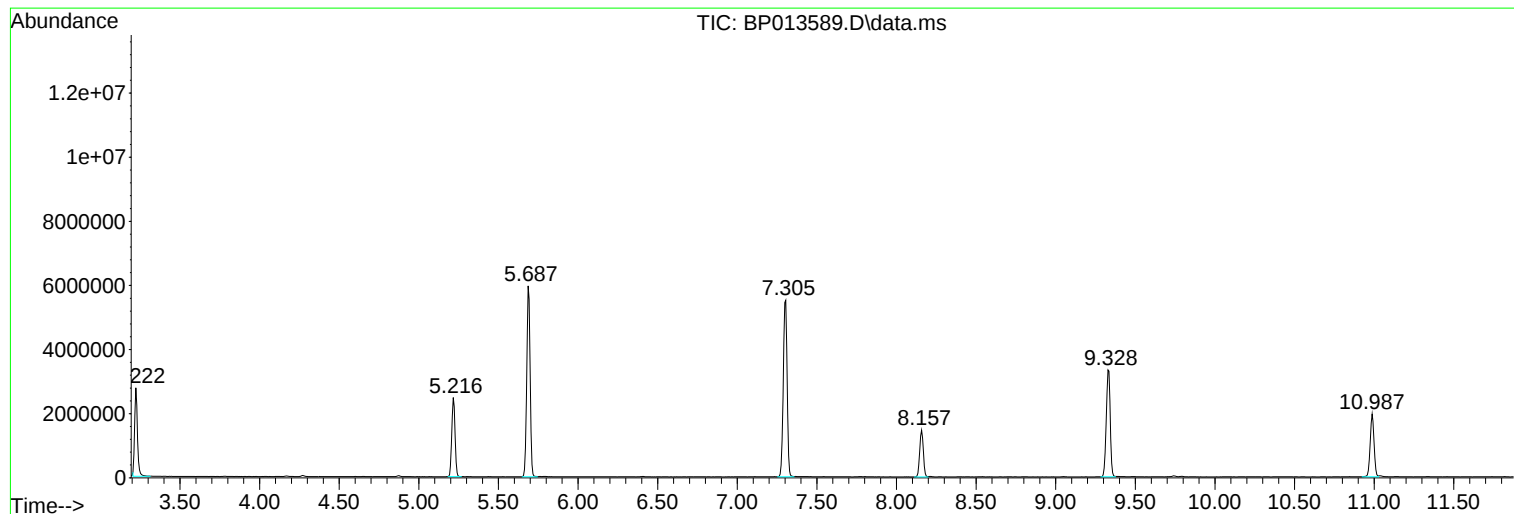
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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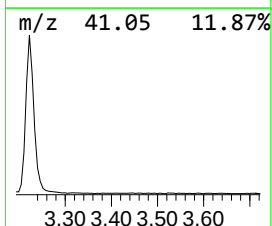
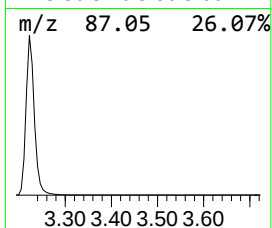
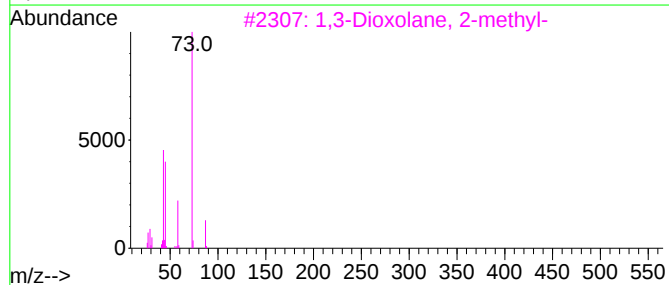
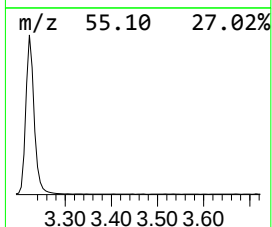
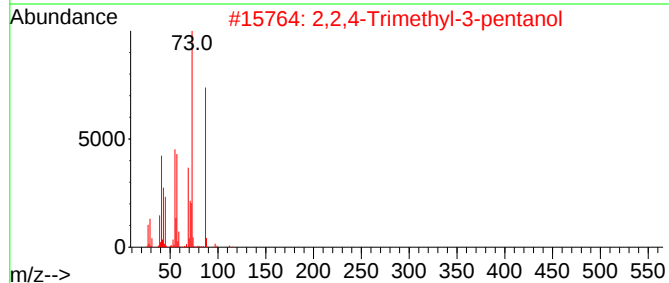
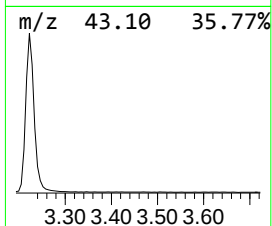
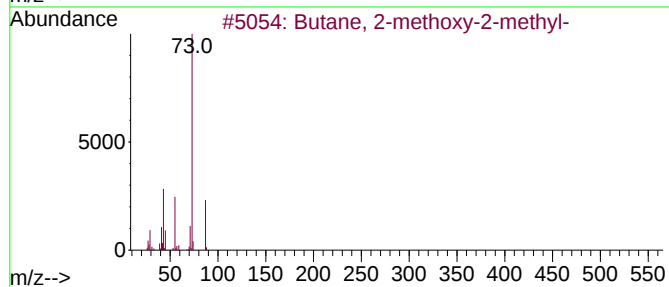
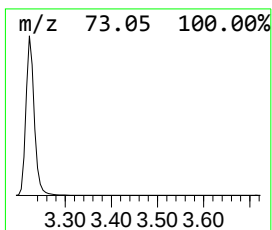
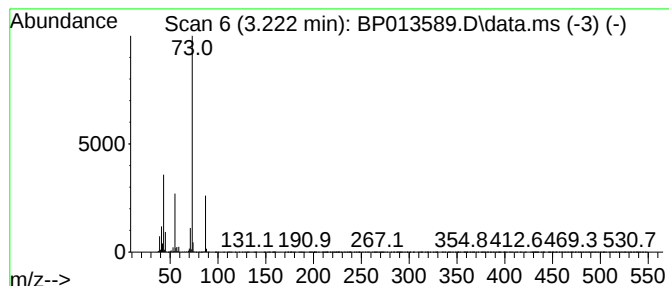
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.222	29.56 ng	3395860	1,4-Dichlorobenzene-d4	8.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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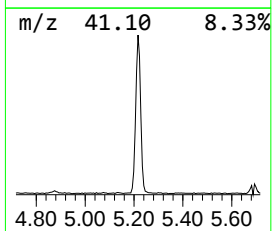
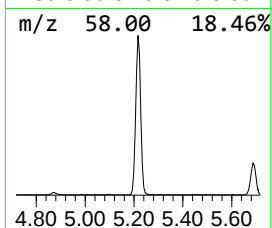
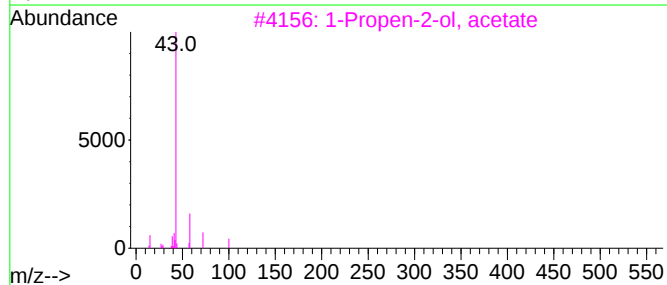
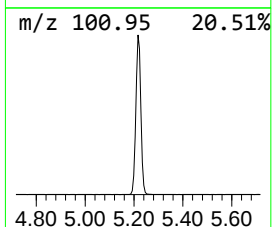
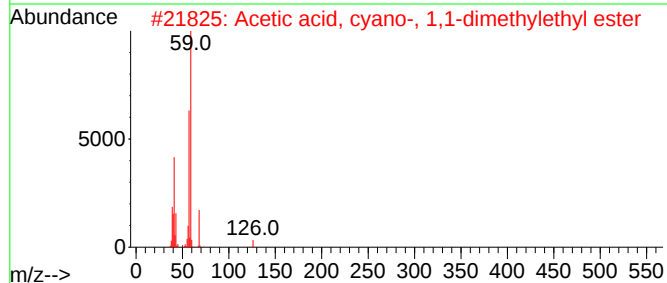
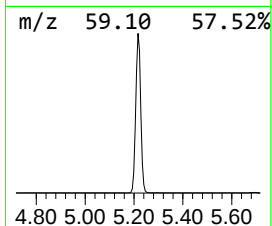
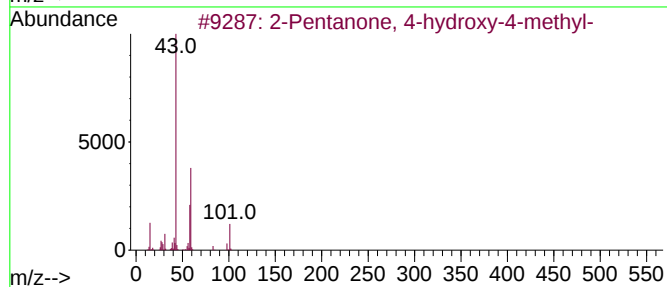
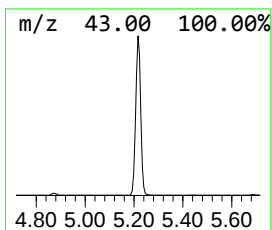
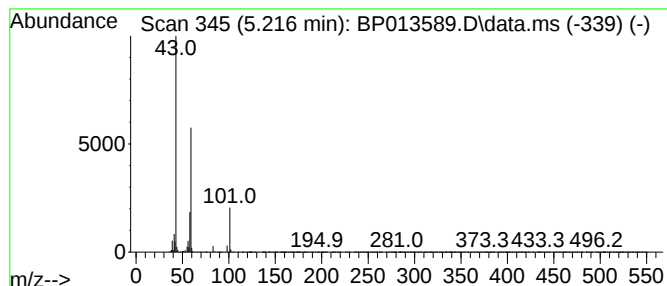
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.216	30.01 ng	3447670	1,4-Dichlorobenzene-d4	8.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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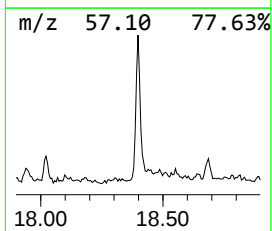
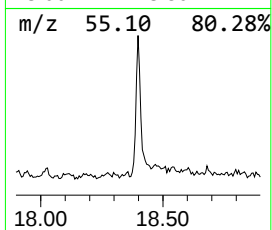
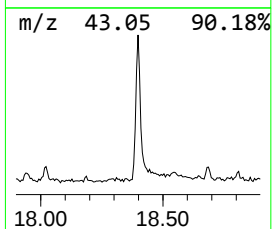
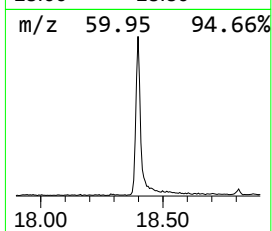
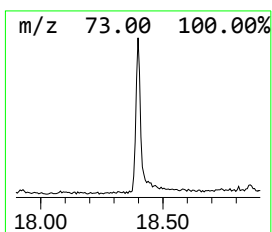
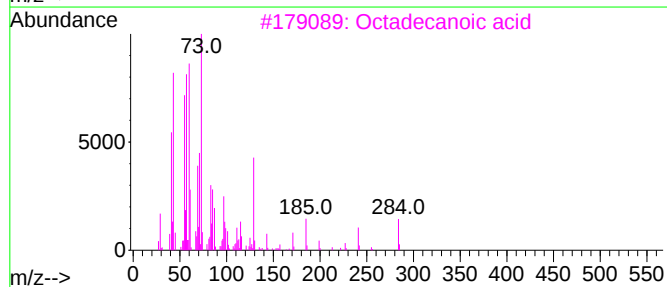
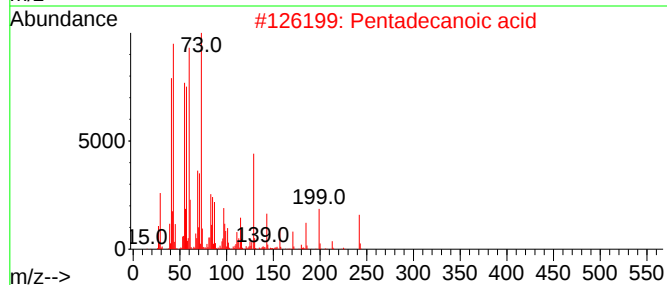
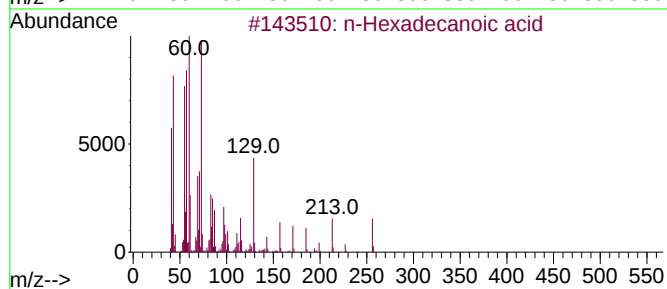
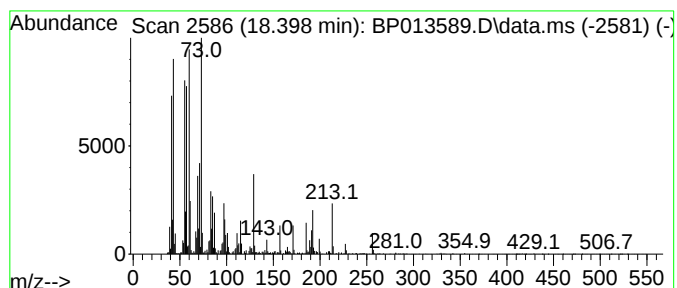
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.398	2.29 ng	568373	Phenanthrene-d10	17.545	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Octadecanoic acid	284	C18H36O2	000057-11-4	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Undecanoic acid	186	C11H22O2	000112-37-8	76



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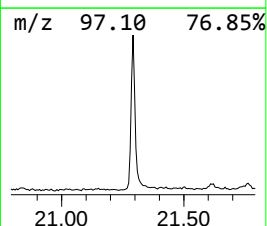
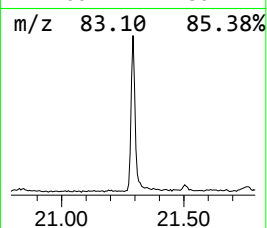
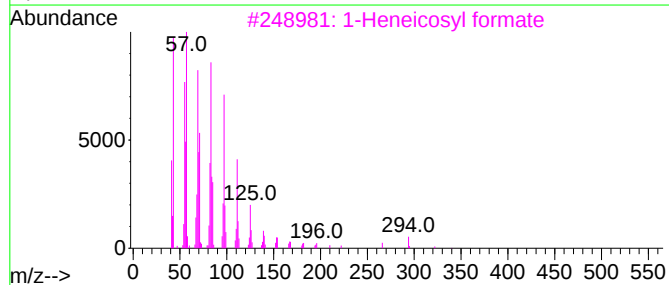
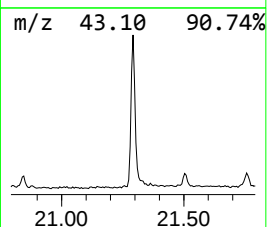
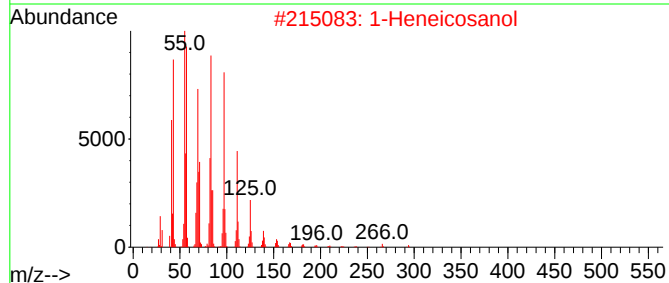
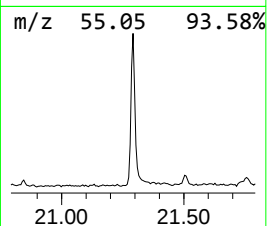
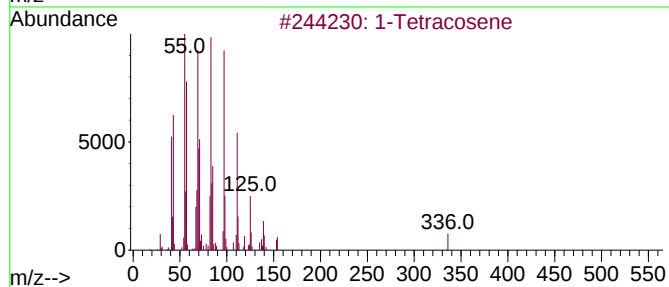
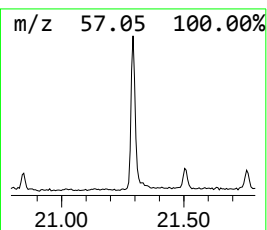
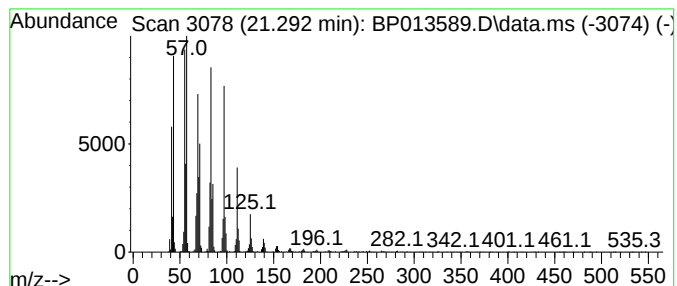
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Peak Number 4 1-Tetracosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.292	6.42 ng	1346260	Chrysene-d12	21.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tetracosene	336	C24H48	010192-32-2	95
2			1-Heneicosanol	312	C21H44O	015594-90-8	95
3			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4			Pentacos-1-ene	350	C25H50	016980-85-1	94
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.222	29.6	ng	3395860	1	8.157	2297460	20.0
2-Pentanone, 4-...	5.216	30.0	ng	3447670	1	8.157	2297460	20.0
n-Hexadecanoic ...	18.398	2.3	ng	568373	4	17.545	4972180	20.0
1-Tetracosene	21.292	6.4	ng	1346260	5	21.616	4192190	20.0