

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082621\
 Data File : BF125235.D
 Acq On : 26 Aug 2021 20:43
 Operator : JU/CG
 Sample : M3546-03
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TRP-7-COMP

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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125235.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	17	24	32	rVB	975686	1253787	27.62%	3.713%
2	5.534	581	586	589	rBV	4283058	4046069	89.12%	11.983%
3	6.534	751	756	759	rBV	4031719	4014802	88.43%	11.890%
4	6.910	817	820	824	rBV	1475307	1224596	26.97%	3.627%
5	7.475	911	916	919	rBV	2887394	2599255	57.25%	7.698%
6	8.092	1018	1021	1035	rBV	232094	411168	9.06%	1.218%
7	8.192	1035	1038	1042	rVV	1805141	1558183	34.32%	4.615%
8	9.269	1216	1221	1224	rBV	5407193	4539986	100.00%	13.446%
9	9.951	1333	1337	1347	rVB	1861335	1762488	38.82%	5.220%
10	10.733	1466	1470	1487	rVB	3173784	3010334	66.31%	8.916%
11	11.433	1585	1589	1593	rBV	1999832	1762298	38.82%	5.219%
12	11.951	1671	1677	1682	rBV2	204384	223316	4.92%	0.661%
13	12.645	1792	1795	1802	rBV	79240	77087	1.70%	0.228%
14	12.739	1808	1811	1816	rBV2	47691	56951	1.25%	0.169%
15	12.874	1829	1834	1838	rBV	84959	95932	2.11%	0.284%
16	13.021	1854	1859	1862	rBV	4472580	4136524	91.11%	12.251%
17	14.074	2031	2038	2041	rBV	1384070	1275922	28.10%	3.779%
18	14.833	2164	2167	2173	rBV2	102789	143955	3.17%	0.426%
19	15.127	2213	2217	2220	rBV	47615	79988	1.76%	0.237%
20	15.439	2266	2270	2276	rBV	36948	56326	1.24%	0.167%
21	15.504	2277	2281	2286	rVV	45718	64819	1.43%	0.192%
22	15.568	2287	2292	2304	rVB	1054762	1371084	30.20%	4.061%

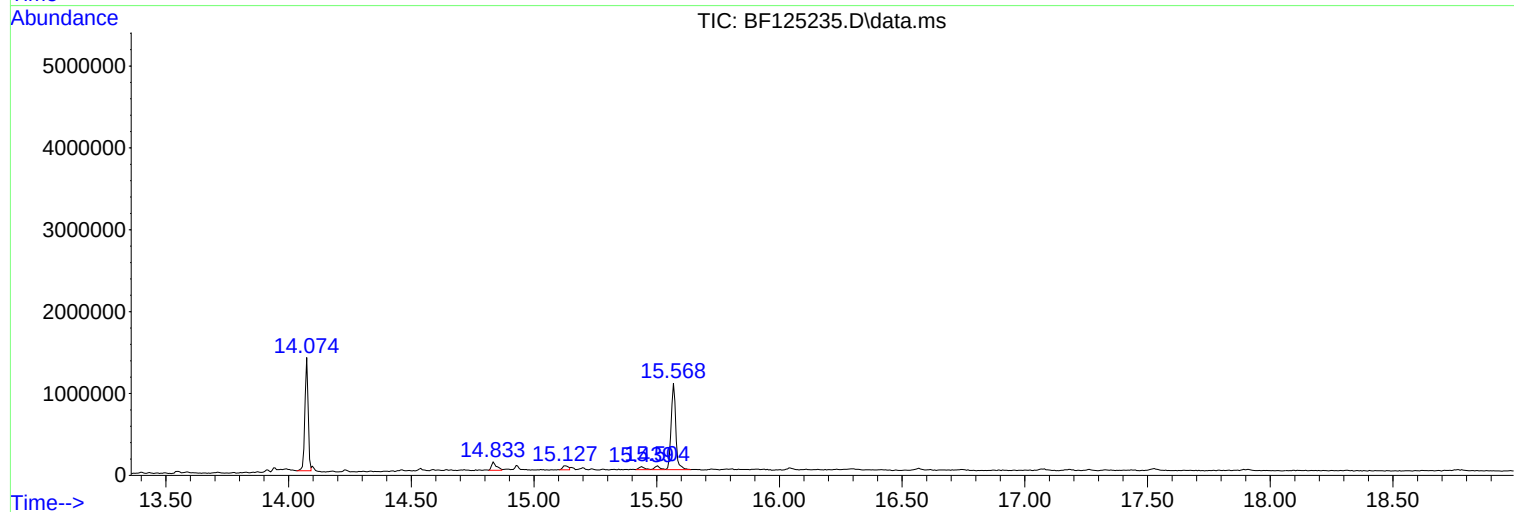
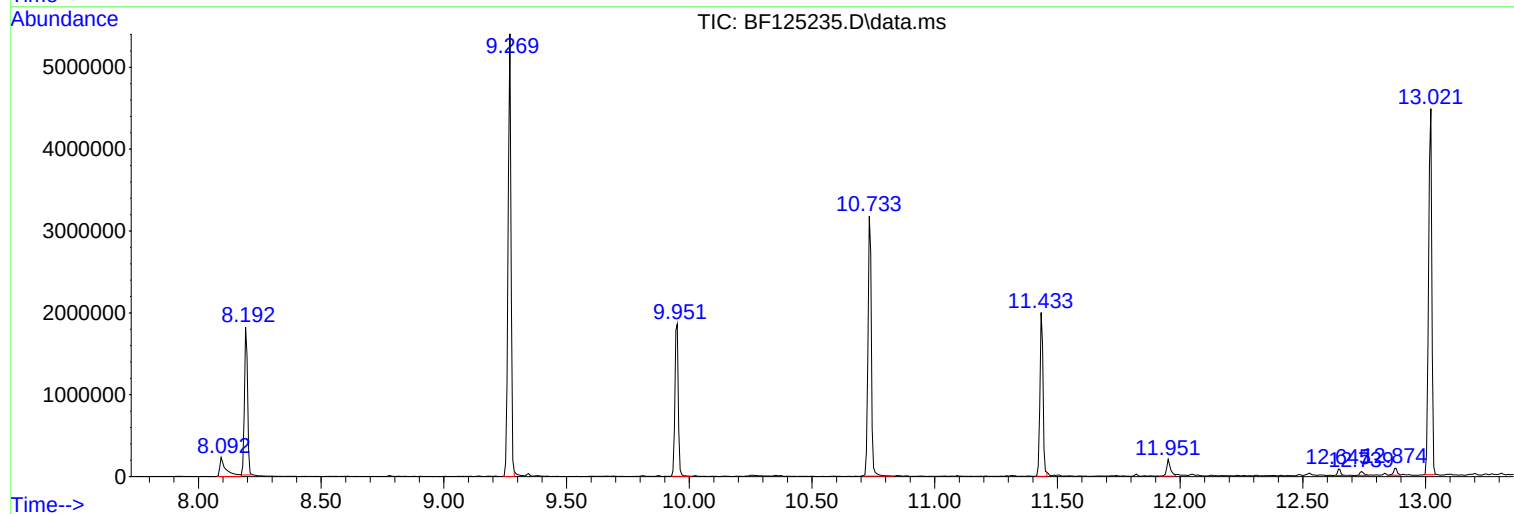
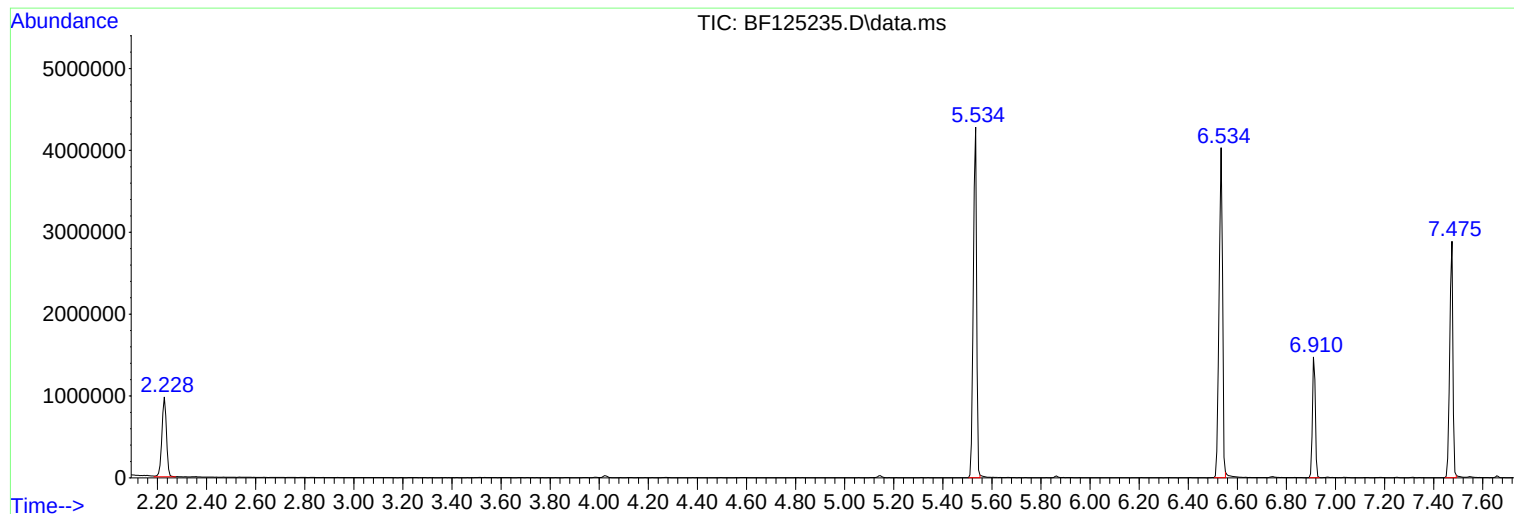
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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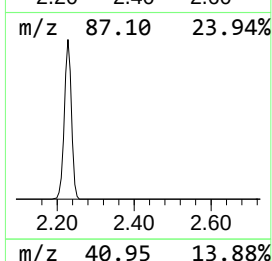
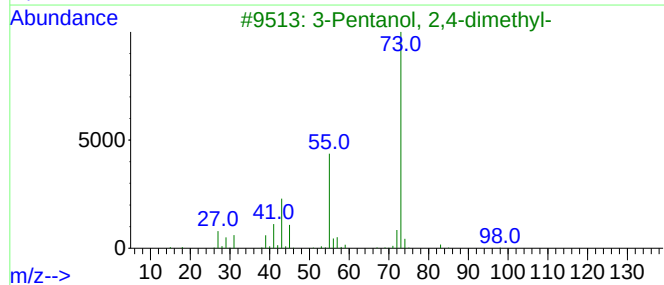
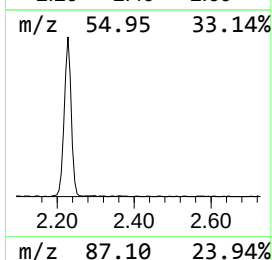
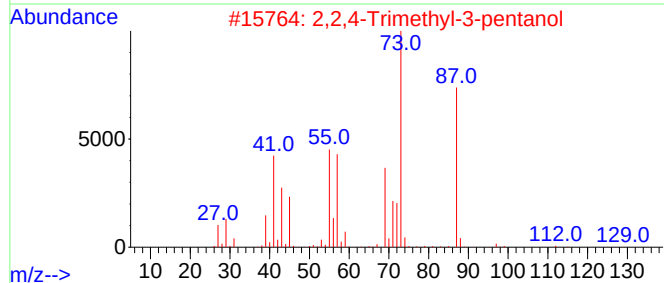
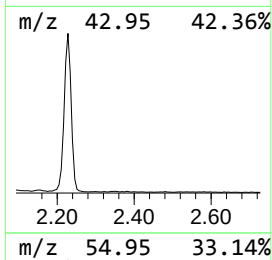
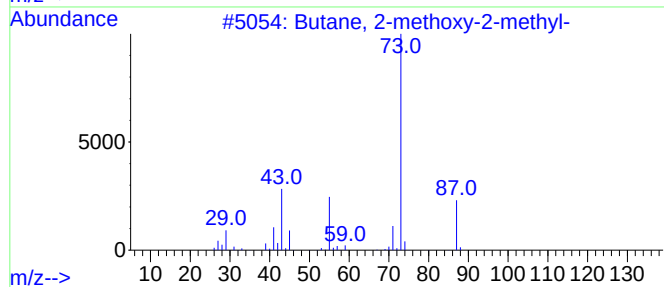
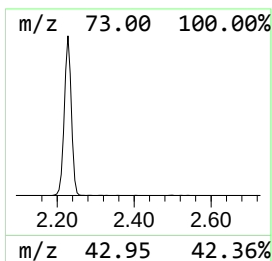
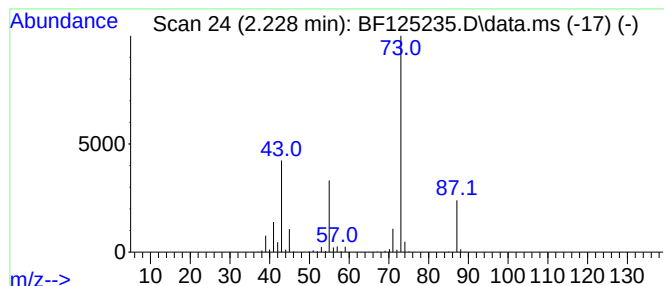
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	20.48 ng	1253790	1,4-Dichlorobenzene-d4	6.910

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	40
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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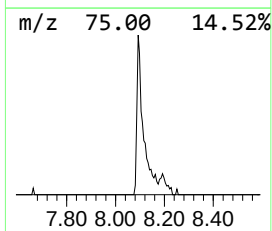
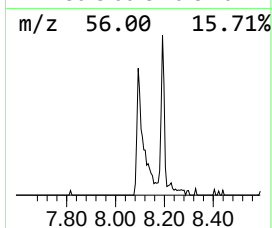
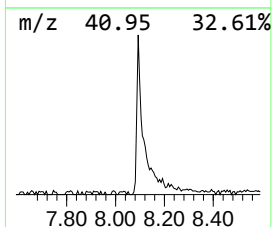
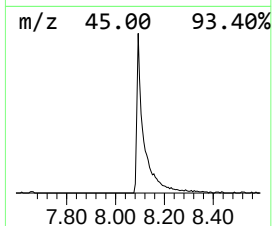
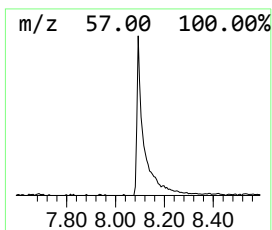
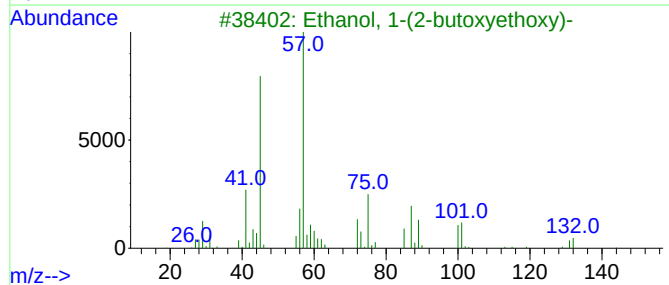
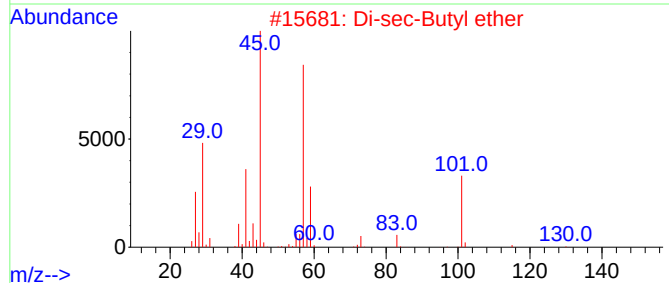
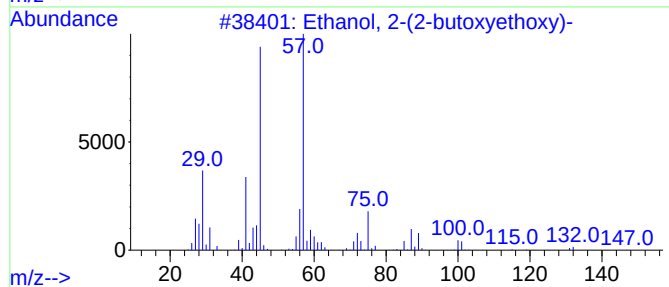
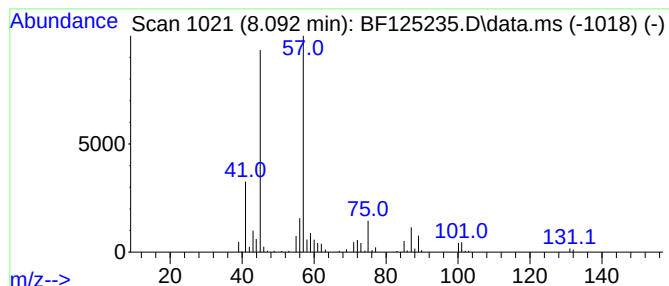
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	5.28 ng	411168	Naphthalene-d8	8.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
3			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



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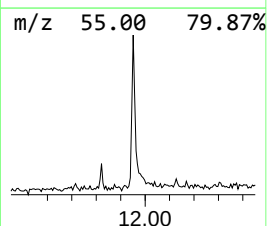
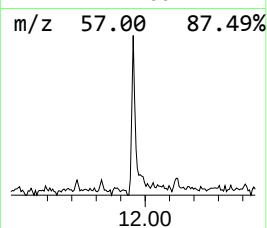
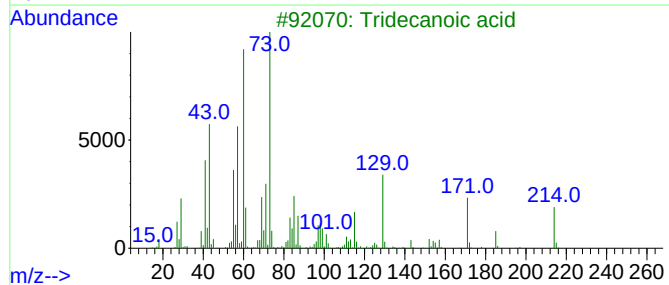
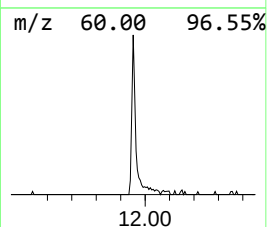
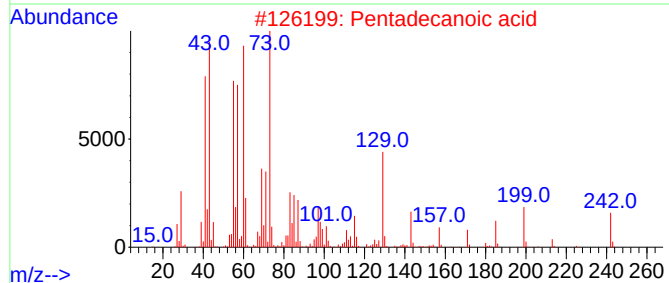
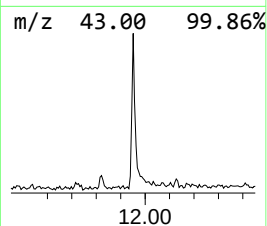
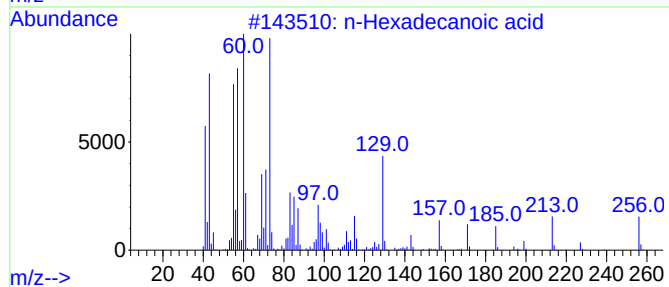
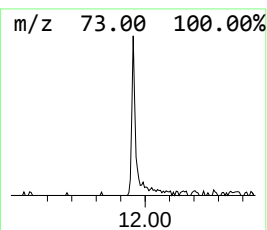
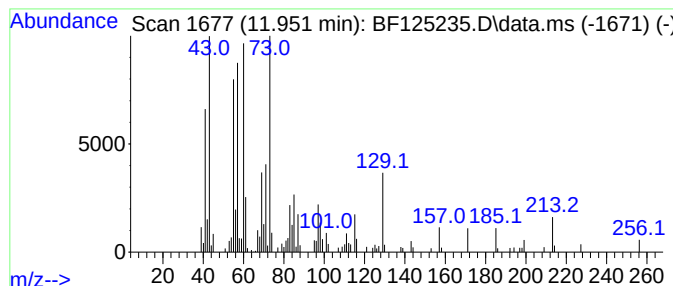
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	2.53 ng	223316	Phenanthrene-d10	11.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	83
4			Nonanoic acid	158	C9H18O2	000112-05-0	43
5			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	35



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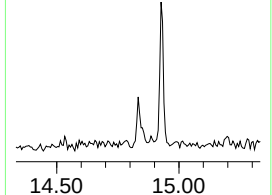
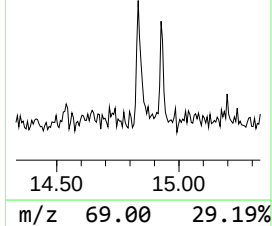
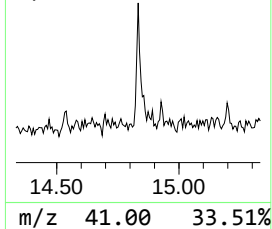
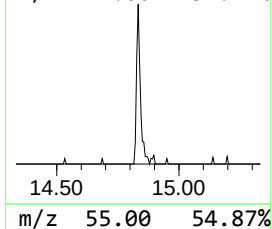
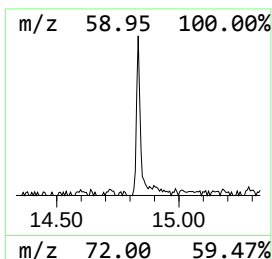
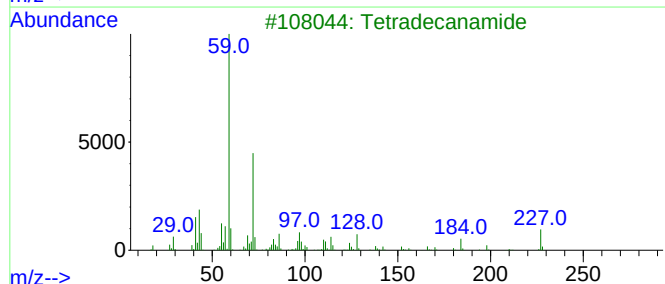
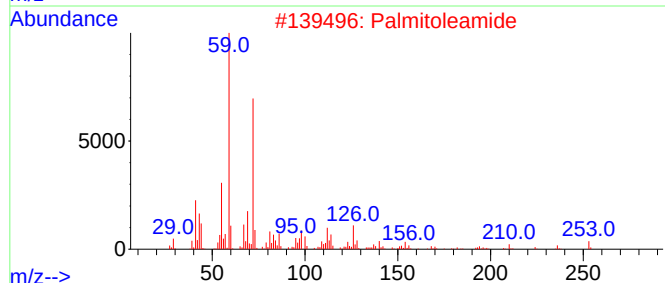
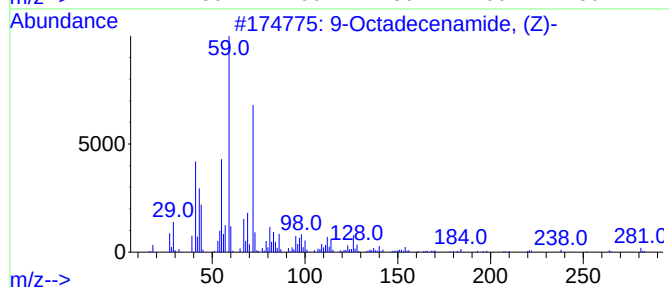
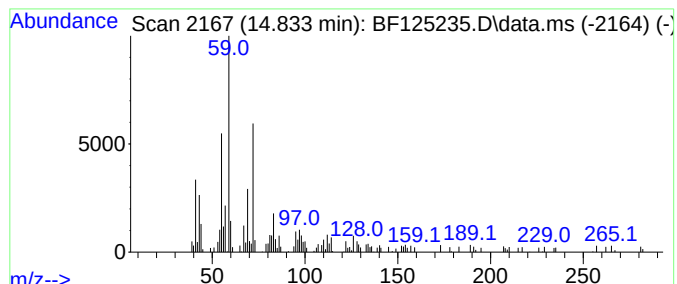
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Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	2.10 ng	143955	Perylene-d12	15.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2			Palmitoleamide	253	C16H31NO	106010-22-4	80
3			Tetradecanamide	227	C14H29NO	000638-58-4	72
4			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59
5			Dodecanamide	199	C12H25NO	001120-16-7	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.228	20.5	ng	1253790	1	6.910	1224600	20.0
Ethanol, 2-(2-b...	8.092	5.3	ng	411168	2	8.192	1558180	20.0
n-Hexadecanoic ...	11.951	2.5	ng	223316	4	11.433	1762300	20.0
9-Octadecenamid...	14.833	2.1	ng	143955	6	15.568	1371080	20.0