

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
 Data File : BF125932.D
 Acq On : 26 Oct 2021 13:46
 Operator : JU/CG
 Sample : M4325-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RED-BOX-2-1934

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-BF102521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125932.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	7	16	22	rVB	3314304	4522346	74.60%	9.888%
2	3.369	214	218	227	rBV	34538	70678	1.17%	0.155%
3	5.110	511	514	520	rVB	49429	68105	1.12%	0.149%
4	5.487	572	578	581	rBV	5507021	6041849	99.66%	13.210%
5	6.492	742	749	752	rBV	5034766	6062347	100.00%	13.255%
6	6.863	809	812	816	rBV	1024508	897464	14.80%	1.962%
7	7.428	902	908	911	rBV	3781881	4031600	66.50%	8.815%
8	8.051	1010	1014	1018	rBV	1577221	1432782	23.63%	3.133%
9	8.145	1026	1030	1034	rBV	1323324	1191624	19.66%	2.605%
10	9.228	1208	1214	1217	rBV	5906876	5701584	94.05%	12.466%
11	9.904	1325	1329	1332	rVB	1513089	1296280	21.38%	2.834%
12	10.692	1456	1463	1466	rBV	4473979	4200150	69.28%	9.183%
13	11.386	1577	1581	1584	rBV	1723962	1380853	22.78%	3.019%
14	11.457	1587	1593	1596	rVB3	83136	75873	1.25%	0.166%
15	11.916	1665	1671	1676	rBV	241412	224658	3.71%	0.491%
16	12.704	1801	1805	1812	rBV2	67469	99680	1.64%	0.218%
17	12.980	1847	1852	1855	rBV	6011126	6032004	99.50%	13.188%
18	13.874	1999	2004	2011	rBV2	224618	263273	4.34%	0.576%
19	14.021	2025	2029	2033	rBV	1229740	1202769	19.84%	2.630%
20	14.898	2175	2178	2181	rVB	110192	99529	1.64%	0.218%
21	15.492	2274	2279	2285	rBV2	722263	842075	13.89%	1.841%

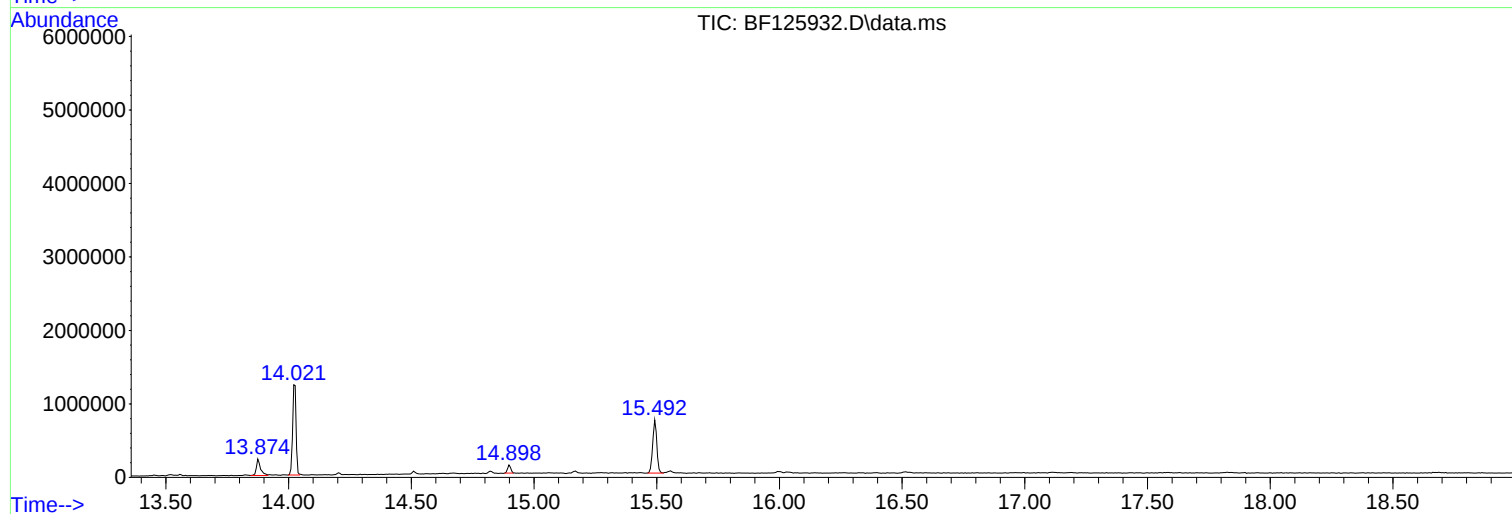
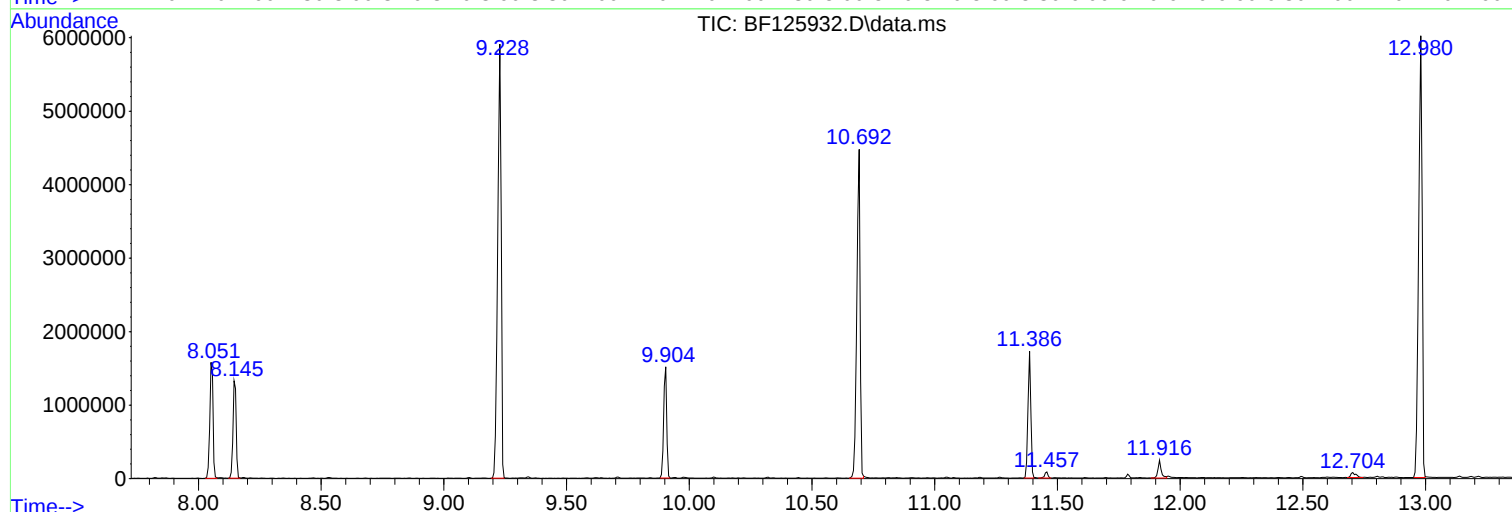
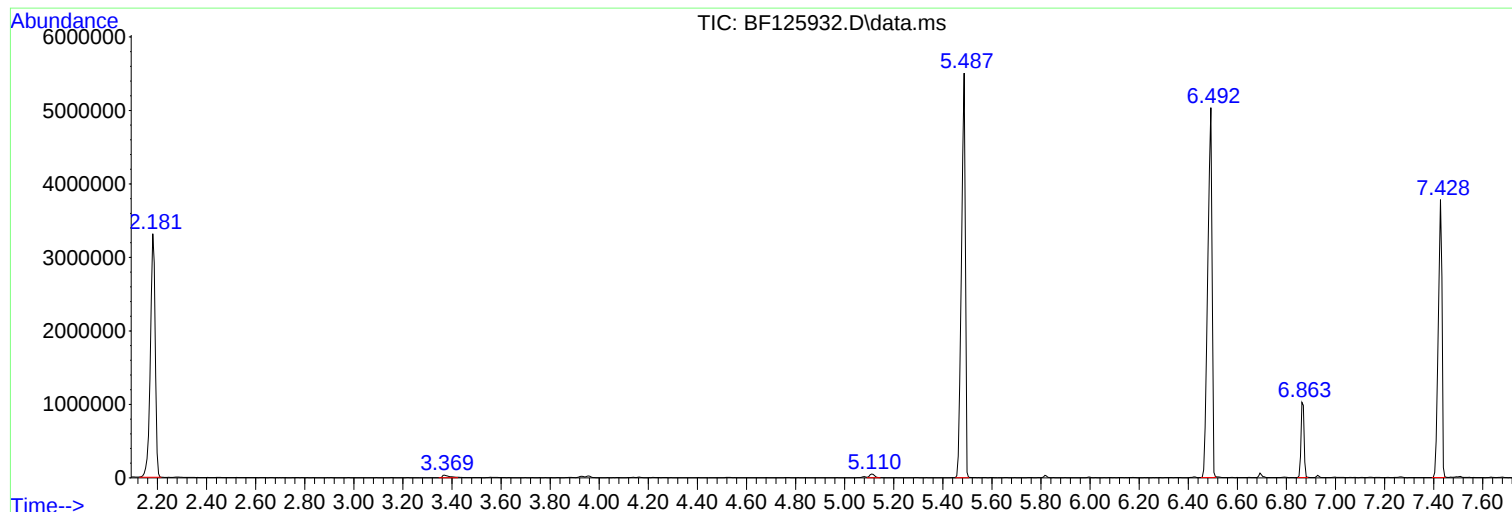
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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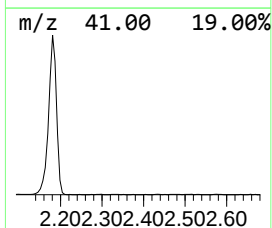
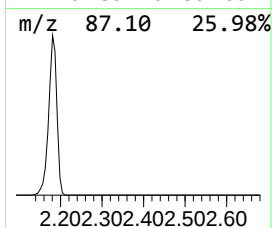
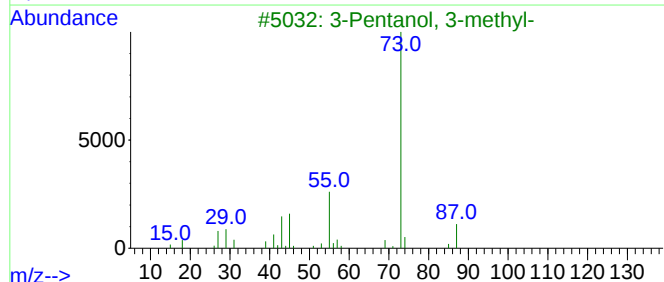
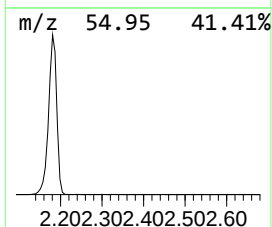
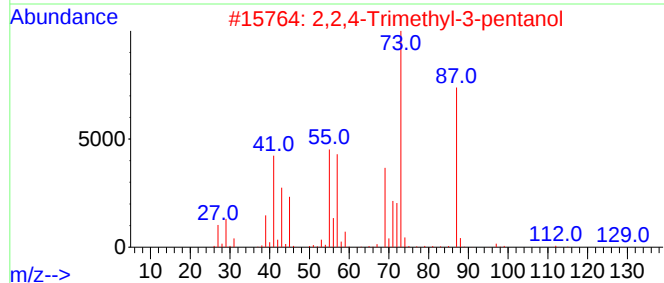
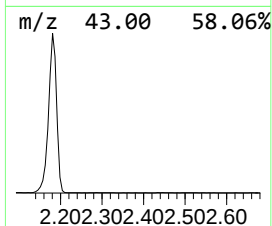
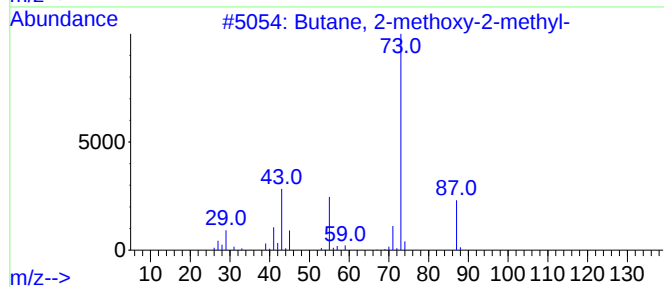
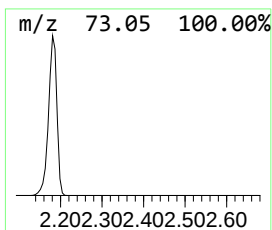
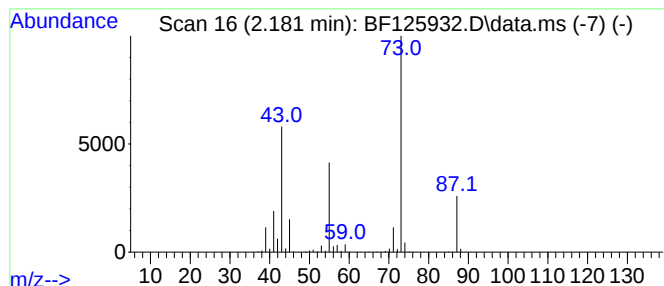
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	100.78 ng	4522350	1,4-Dichlorobenzene-d4	6.869

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			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	32
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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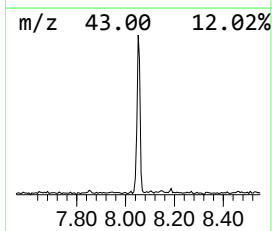
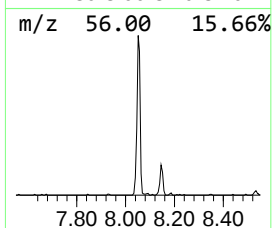
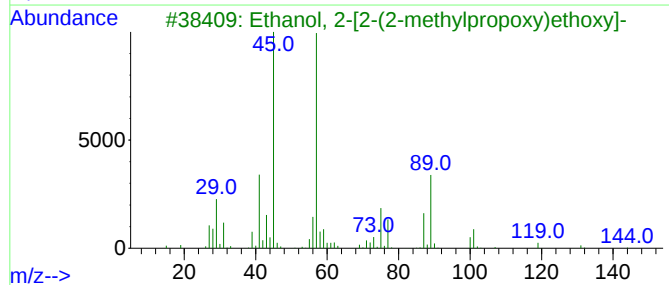
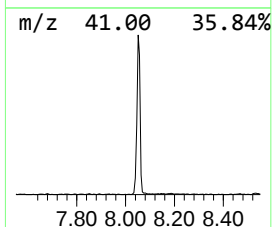
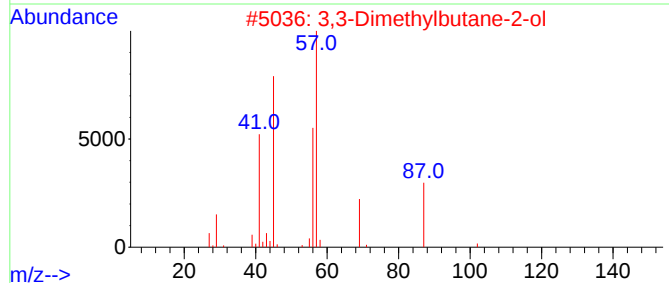
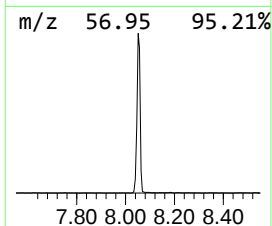
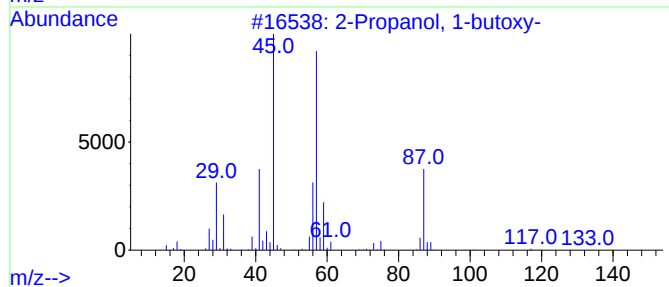
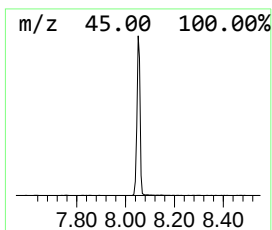
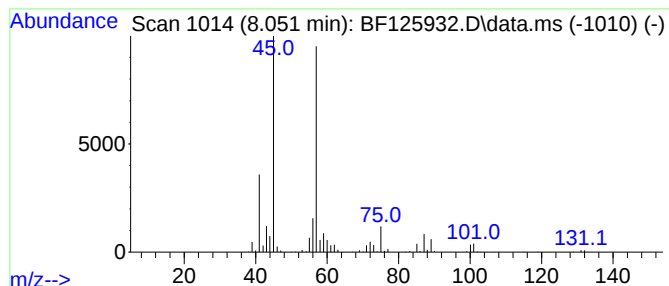
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Propanol, 1-butoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	24.05 ng	1432780	Naphthalene-d8	8.145

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	59	
2	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53	
3	Ethanol, 2-[2-(2-methylpropoxy)ethoxy]-	162	C8H18O3	018912-80-6	50	
4	Butyl lactate	146	C7H14O3	000138-22-7	50	
5	2-Hexanol	102	C6H14O	000626-93-7	47	



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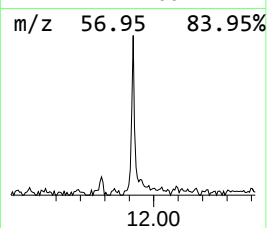
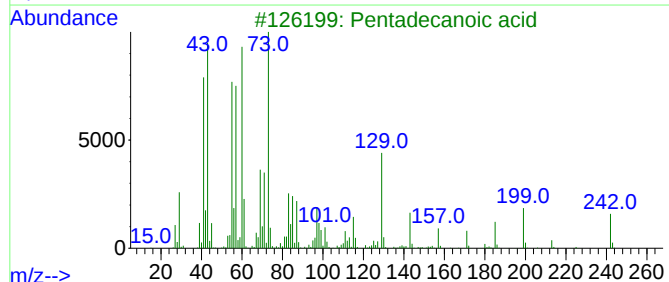
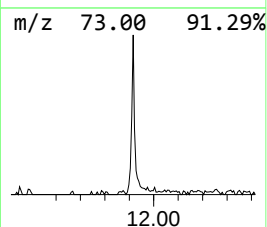
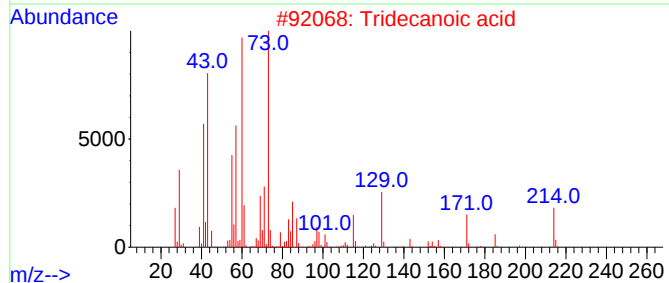
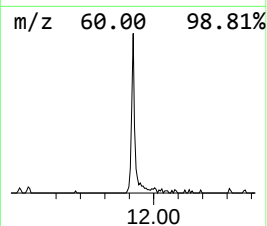
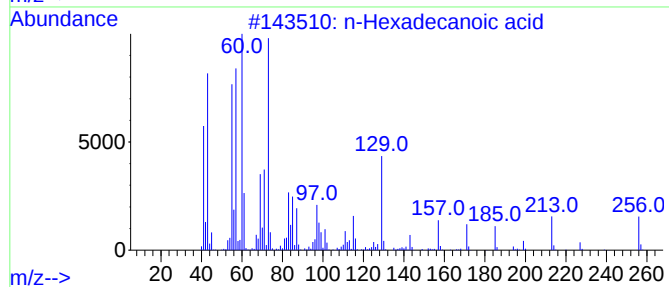
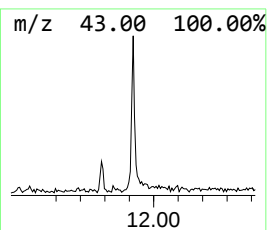
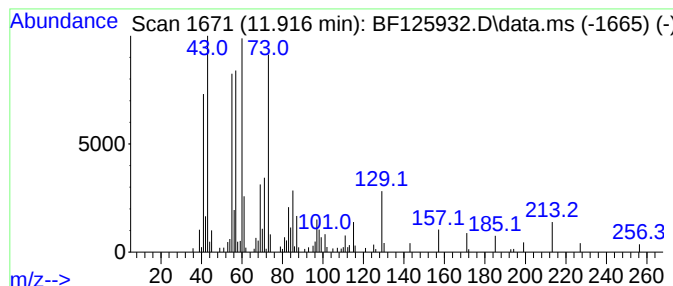
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	3.25 ng	224658	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2			Tridecanoic acid	214	C13H26O2	000638-53-9	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4			Undecanoic acid	186	C11H22O2	000112-37-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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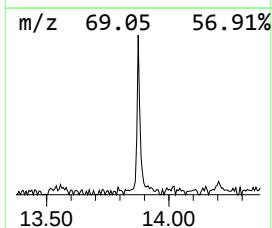
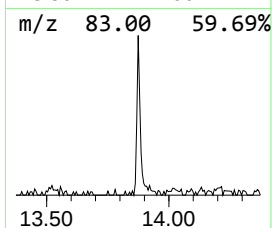
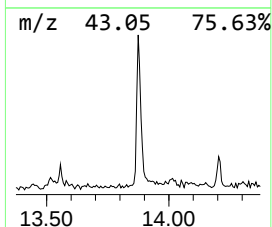
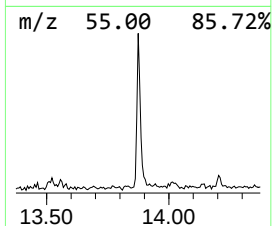
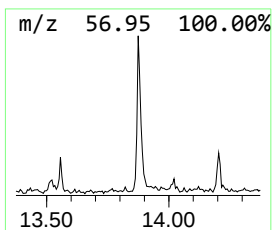
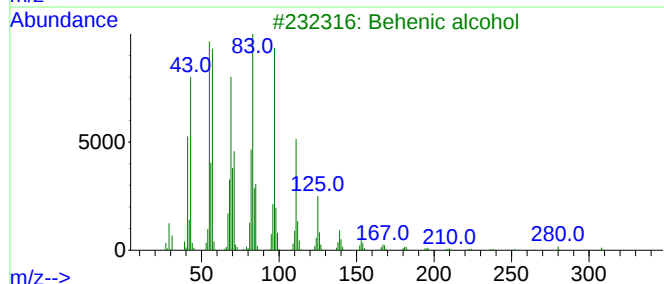
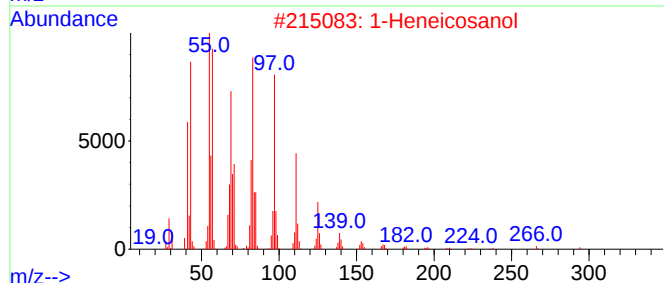
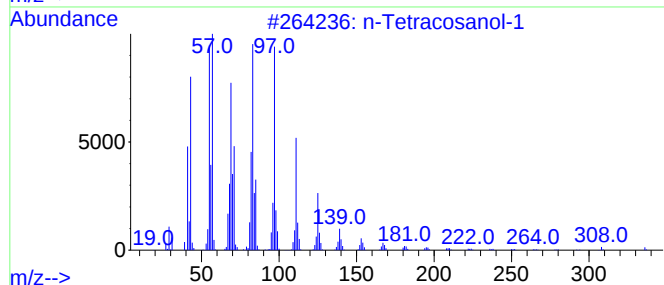
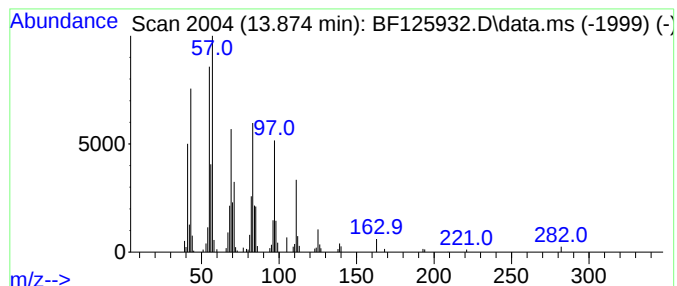
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Peak Number 4 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	4.38 ng	263273	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2			1-Heneicosanol	312	C21H44O	015594-90-8	90
3			Behenic alcohol	326	C22H46O	000661-19-8	87
4			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	87
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	86



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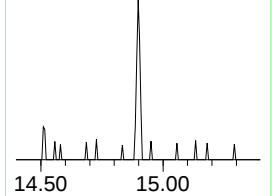
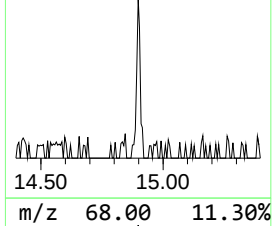
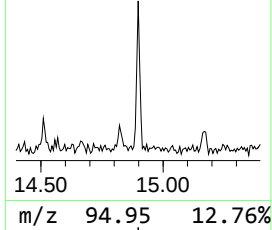
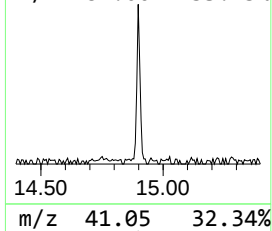
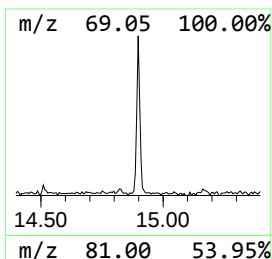
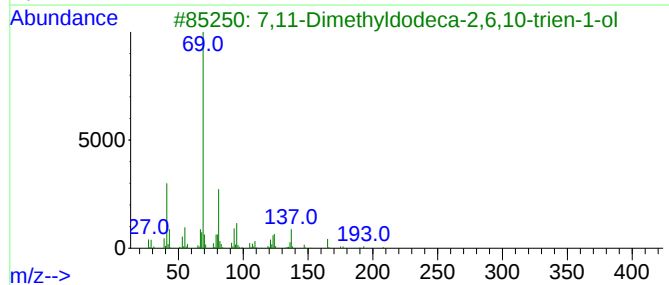
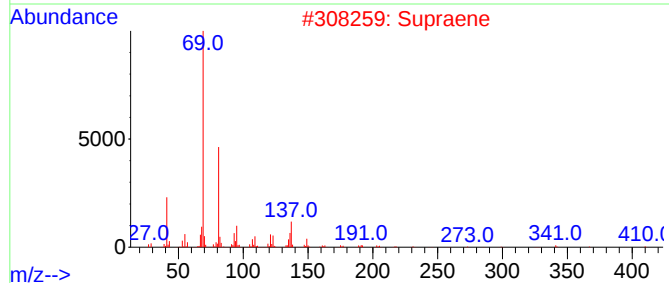
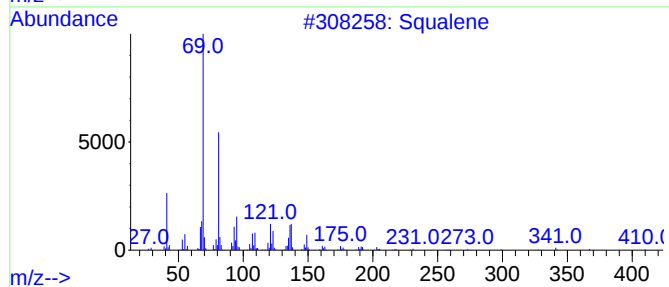
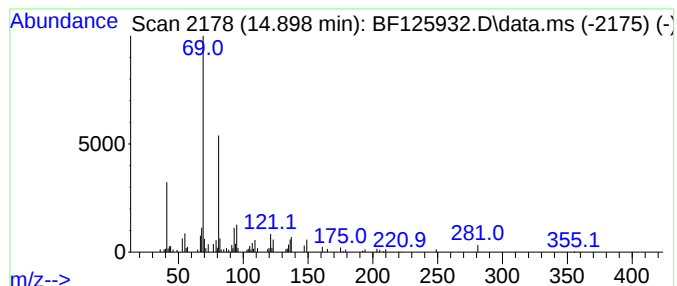
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Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	2.36 ng	99529	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	86
2			Supraene	410	C30H50	007683-64-9	72
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4			2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	64
5			2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.181	100.8	ng	4522350	1	6.869	897464	20.0
2-Propanol, 1-b...	8.051	24.1	ng	1432780	2	8.145	1191620	20.0
n-Hexadecanoic ...	11.916	3.3	ng	224658	4	11.386	1380850	20.0
n-Tetracosanol-1	13.874	4.4	ng	263273	5	14.027	1202770	20.0
Squalene	14.898	2.4	ng	99529	6	15.492	842075	20.0