

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
 Data File : BF126067.D
 Acq On : 8 Nov 2021 16:09
 Operator : JU/CG
 Sample : M4540-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-2

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-BF110321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126067.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	8	16	27	rVB	1950540	2489375	55.99%	8.120%
2	5.475	571	576	579	rBV	4397268	3984563	89.62%	12.998%
3	6.481	741	747	750	rBV	4178670	4067653	91.49%	13.269%
4	6.851	807	810	814	rBV	1240649	1015178	22.83%	3.312%
5	7.416	900	906	909	rBV	2777278	2619963	58.93%	8.546%
6	8.034	1007	1011	1024	rBV	266921	324755	7.30%	1.059%
7	8.134	1024	1028	1032	rBV	1462275	1220997	27.46%	3.983%
8	9.210	1206	1211	1214	rBV	5471217	4445845	100.00%	14.503%
9	9.886	1322	1326	1330	rBV	1556736	1252873	28.18%	4.087%
10	10.675	1456	1460	1463	rBV	2608390	2308136	51.92%	7.529%
11	11.369	1575	1578	1581	rBV	1213283	1060716	23.86%	3.460%
12	12.580	1781	1784	1791	rVB	57726	58249	1.31%	0.190%
13	12.957	1844	1848	1851	rBV	4159799	3397252	76.41%	11.082%
14	13.498	1935	1940	1944	rBV	113220	119782	2.69%	0.391%
15	13.863	1999	2002	2012	rBV2	134344	206899	4.65%	0.675%
16	14.010	2021	2027	2030	rBV	1083523	1045262	23.51%	3.410%
17	15.474	2271	2276	2280	rBV	579744	743236	16.72%	2.424%
18	15.510	2280	2282	2290	rVB4	46894	67260	1.51%	0.219%
19	15.951	2354	2357	2362	rVB3	46848	68507	1.54%	0.223%
20	16.457	2439	2443	2448	rBV2	35020	63837	1.44%	0.208%
21	17.057	2541	2545	2550	rVB8	58352	95157	2.14%	0.310%

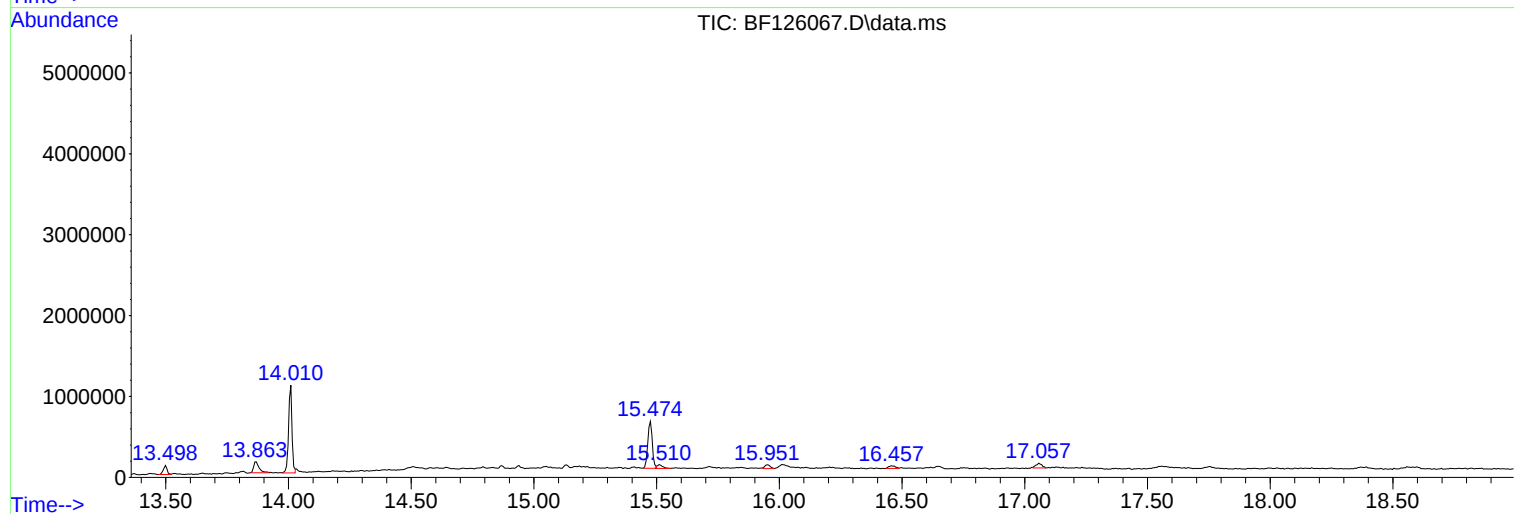
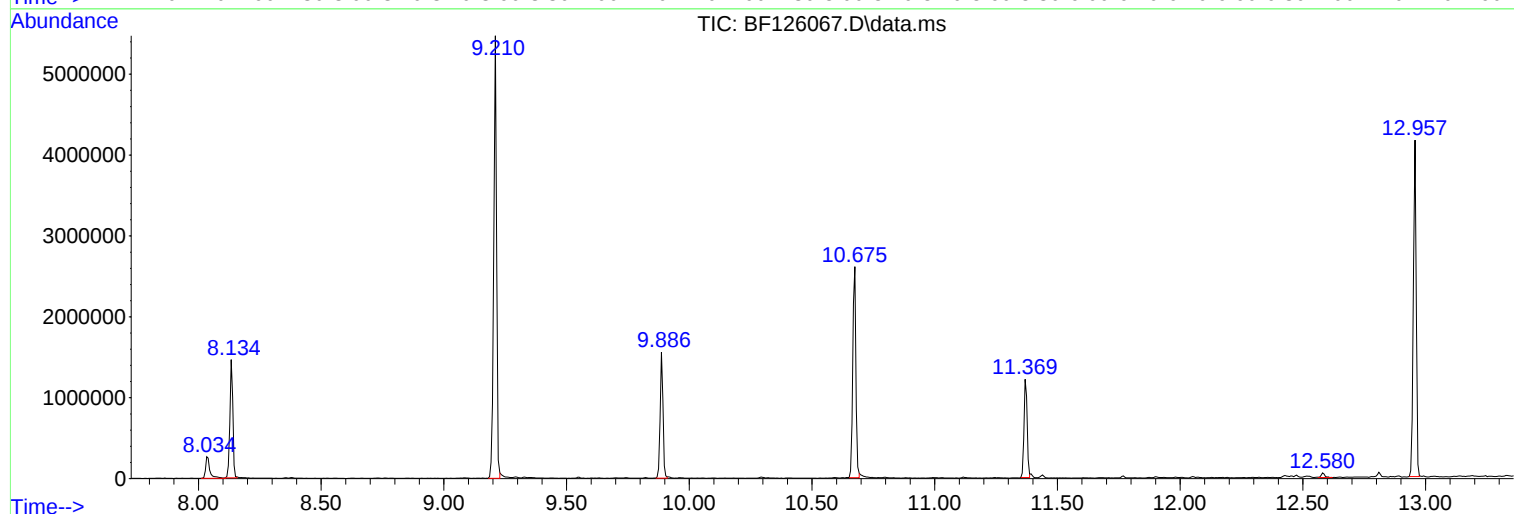
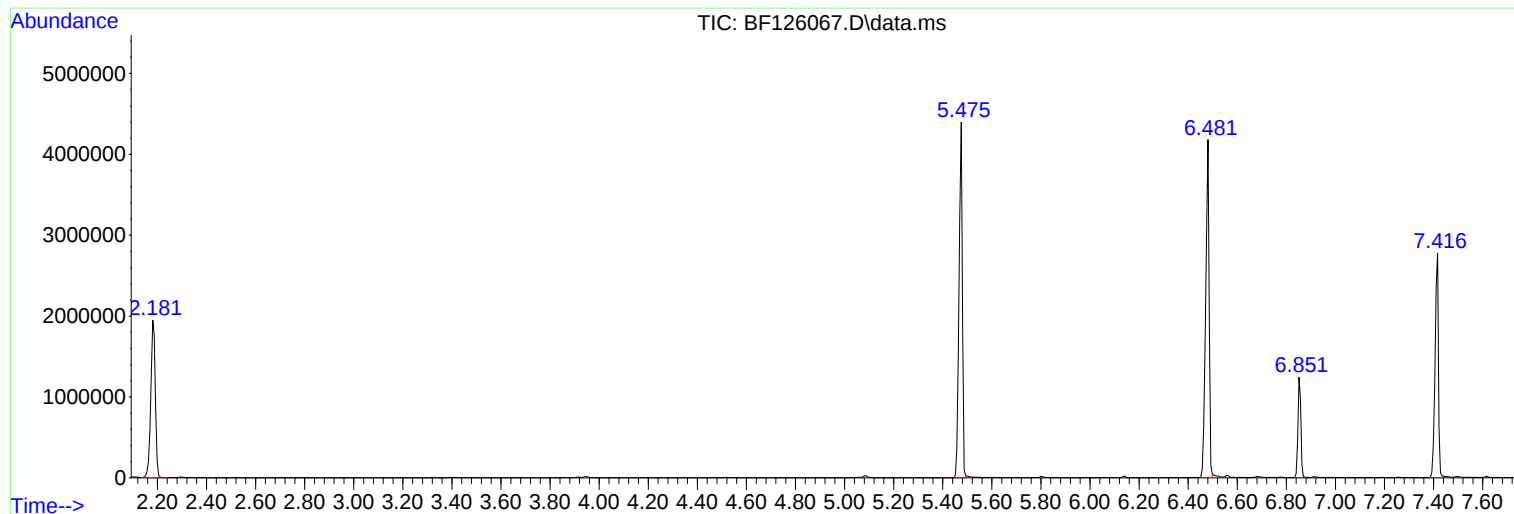
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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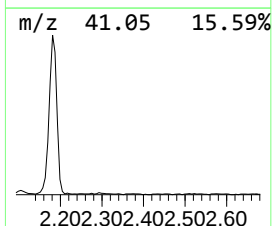
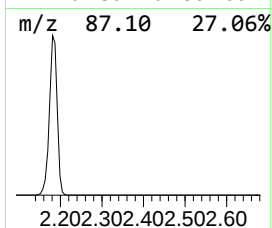
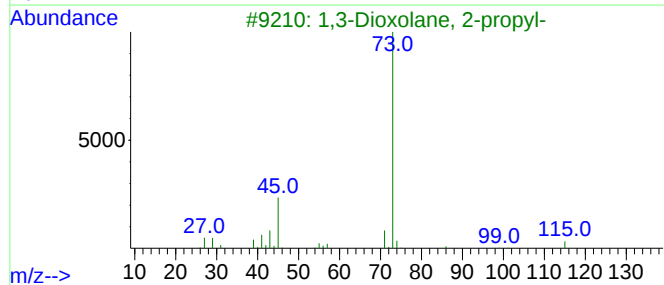
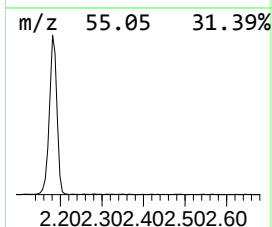
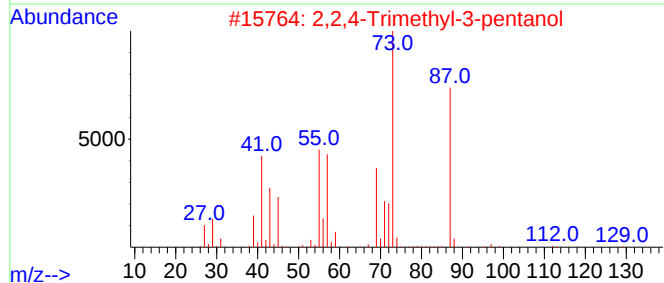
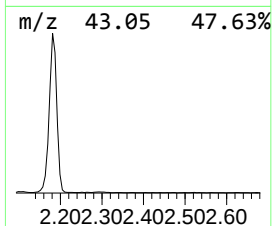
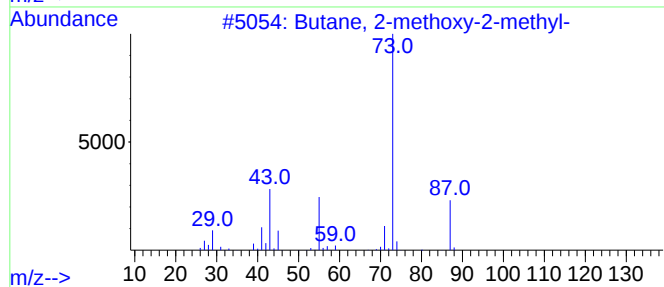
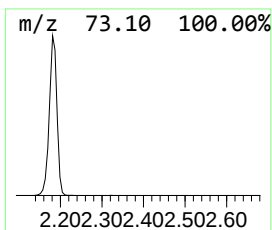
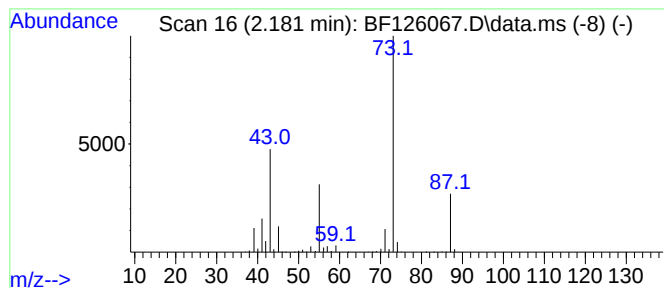
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	49.04 ng	2489380	1,4-Dichlorobenzene-d4	6.851

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			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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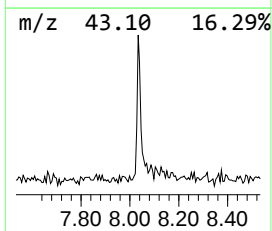
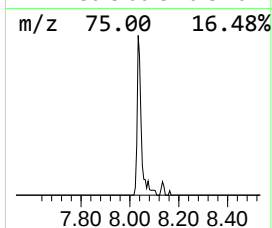
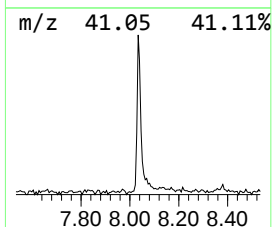
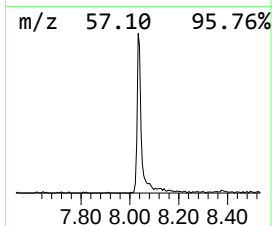
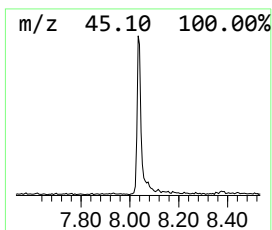
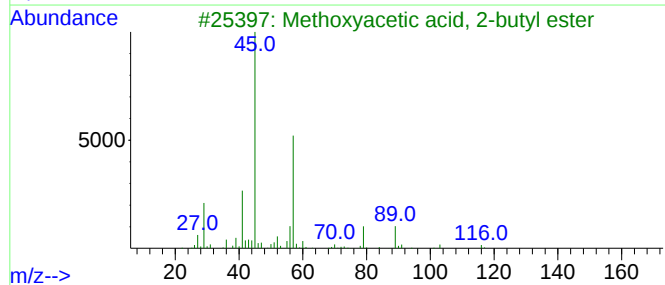
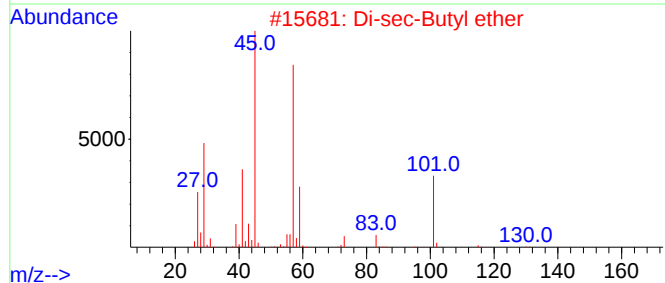
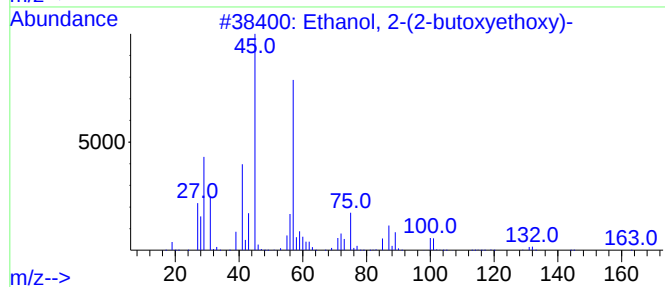
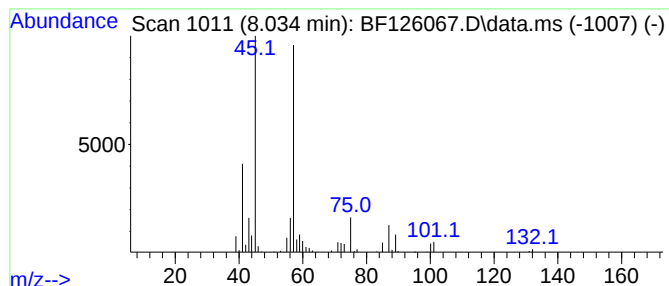
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.034	5.32 ng	324755	Naphthalene-d8	8.134

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
3			Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	53
4			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
5			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50



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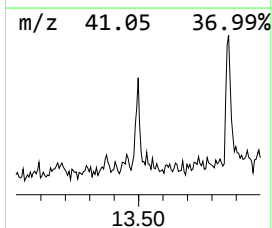
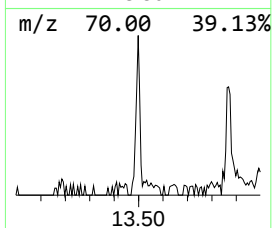
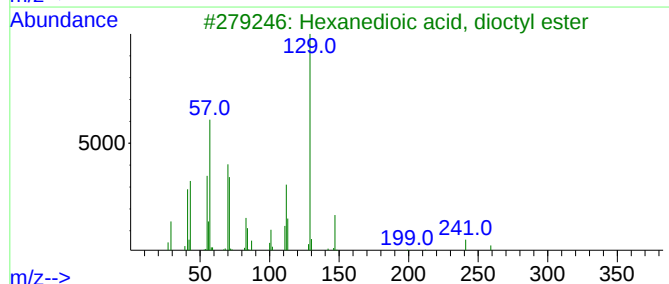
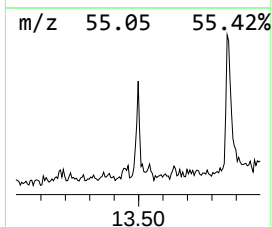
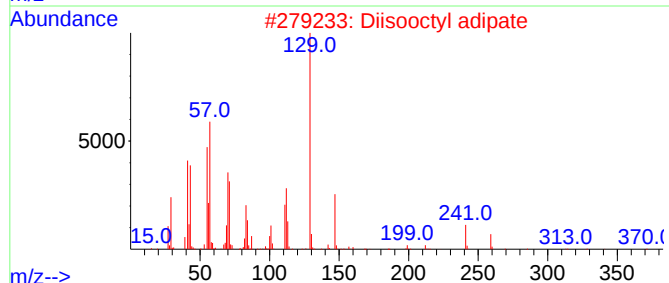
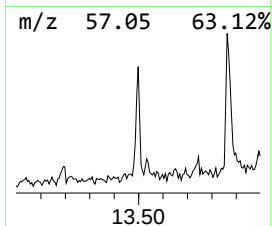
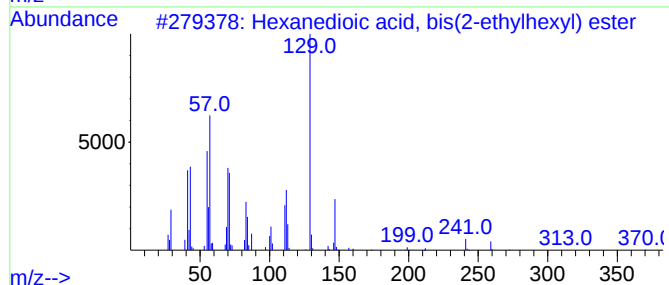
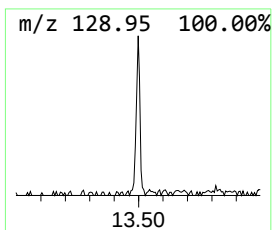
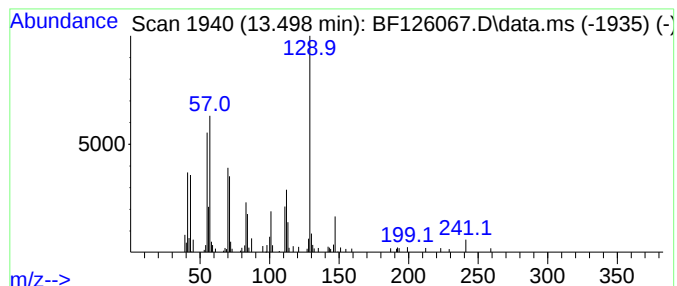
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexanedioic acid, bis(2-eth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.498	2.29 ng	119782	Chrysene-d12	14.010	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	90
2	Diisooctyl adipate	370	C22H42O4	001330-86-5	87
3	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	80
4	Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	72
5	Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1010324-48-0	59



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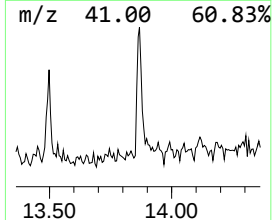
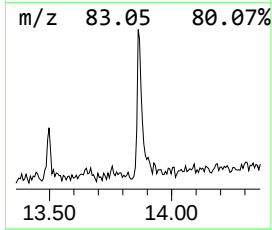
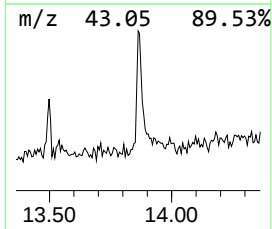
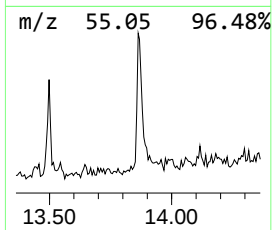
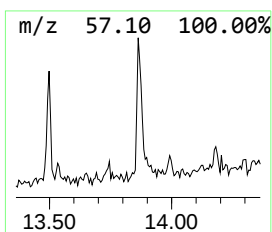
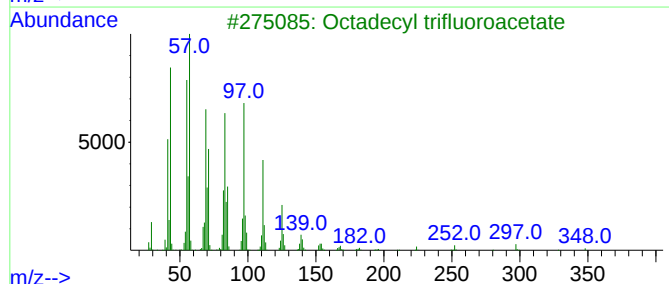
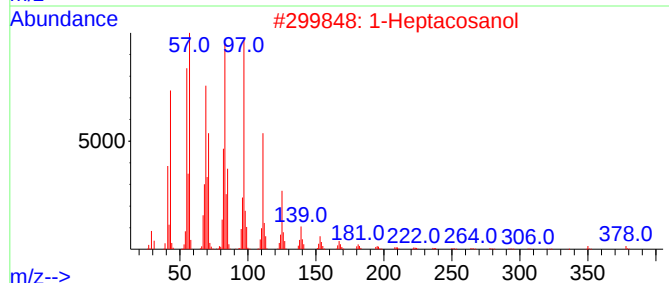
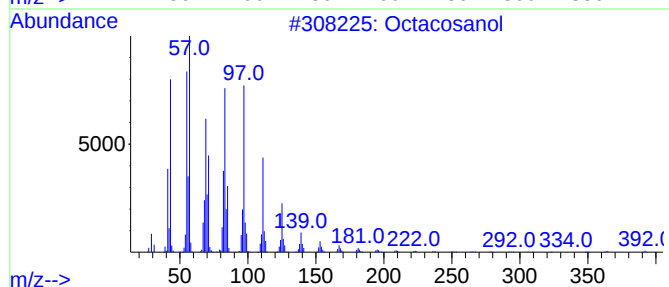
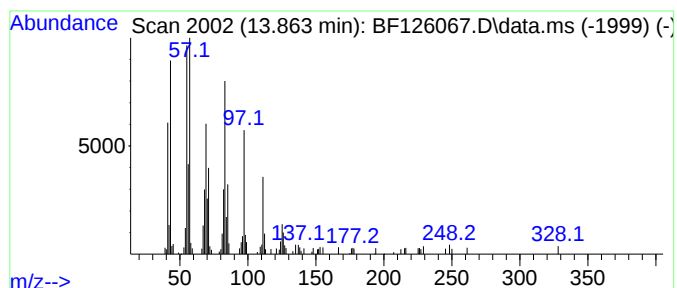
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Peak Number 4 Octacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	3.96 ng	206899	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosanol	410	C28H58O	000557-61-9	90
2			1-Heptacosanol	396	C27H56O	002004-39-9	87
3			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	72
4			17-Pentatriacontene	491	C35H70	006971-40-0	64
5			1-Eicosanol	298	C20H42O	000629-96-9	64



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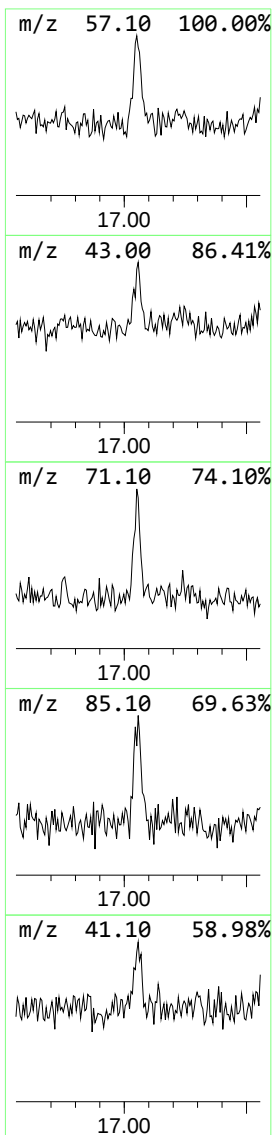
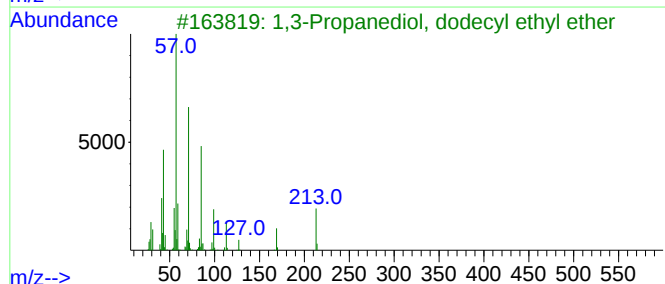
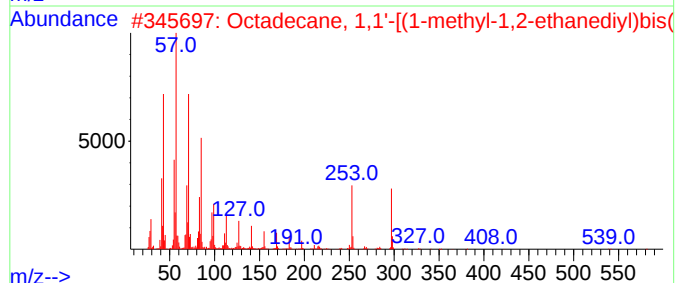
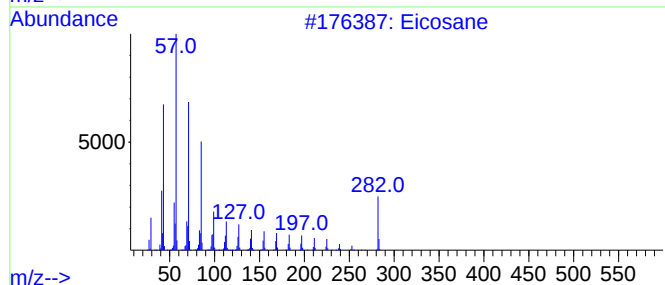
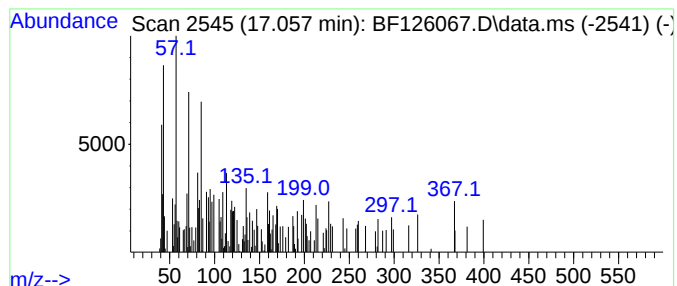
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Peak Number 5 unknown17.057 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.057	2.56 ng	95157	Perylene-d12	15.474	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	38
2	Octadecane, 1,1'-[(1-methyl-1,2-...	581	C39H80O2	035545-51-8	37
3	1,3-Propanediol, dodecyl ethyl e...	272	C17H36O2	1000406-35-1	32
4	Diglycolic acid, decyl 2-methylp...	364	C21H32O5	1000382-01-2	32
5	Oxalic acid, propyl undecyl ester	286	C16H30O4	1000309-26-4	32



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.181	49.0	ng	2489380	1	6.851	1015180	20.0
Ethanol, 2-(2-b...	8.034	5.3	ng	324755	2	8.134	1221000	20.0
Hexanedioic aci...	13.498	2.3	ng	119782	5	14.010	1045260	20.0
Octacosanol	13.863	4.0	ng	206899	5	14.010	1045260	20.0
unknown17.057	17.057	2.6	ng	95157	6	15.474	743236	20.0