

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072722\
 Data File : BF129387.D
 Acq On : 27 Jul 2022 21:04
 Operator : CG\JU
 Sample : N3861-15
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-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_F\Methods\8270-BF072522.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129387.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.122	479	482	491	rVB	86890	98308	1.13%	0.177%
2	5.510	543	548	551	rBV	4153489	3686124	42.20%	6.648%
3	6.510	714	718	730	rVB	2788307	2621764	30.02%	4.729%
4	6.881	777	781	785	rBV	1906876	1576838	18.05%	2.844%
5	6.939	788	791	794	rBV	97078	95440	1.09%	0.172%
6	7.451	871	878	881	rBV	4715597	5219105	59.75%	9.413%
7	7.557	885	896	903	rVV	344215	570799	6.54%	1.029%
8	7.869	946	949	952	rBV	347487	235028	2.69%	0.424%
9	8.163	994	999	1003	rBV	2210315	2126864	24.35%	3.836%
10	9.245	1173	1183	1186	rBV	8716929	8734287	100.00%	15.753%
11	9.628	1244	1248	1252	rBV2	114518	128928	1.48%	0.233%
12	9.898	1274	1294	1296	rBV	2906835	8313129	95.18%	14.993%
13	9.922	1296	1298	1302	rVB	2704059	2238858	25.63%	4.038%
14	10.722	1426	1434	1437	rBV	5614369	5720942	65.50%	10.318%
15	11.416	1548	1552	1555	rBV	2551345	2170781	24.85%	3.915%
16	11.798	1613	1617	1619	rBV	358464	314772	3.60%	0.568%
17	11.933	1637	1640	1643	rBV	138054	144078	1.65%	0.260%
18	12.504	1734	1737	1749	rVB3	242531	392138	4.49%	0.707%
19	12.586	1749	1751	1757	rVB	166758	160515	1.84%	0.290%
20	13.004	1817	1822	1825	rBV	7796165	7799081	89.29%	14.066%
21	13.898	1970	1974	1979	rBV2	84421	163743	1.87%	0.295%
22	14.057	1997	2001	2005	rBV	1839614	1547386	17.72%	2.791%
23	14.898	2141	2144	2148	rVB	99901	96651	1.11%	0.174%
24	15.545	2249	2254	2266	rVB	990705	1289391	14.76%	2.326%

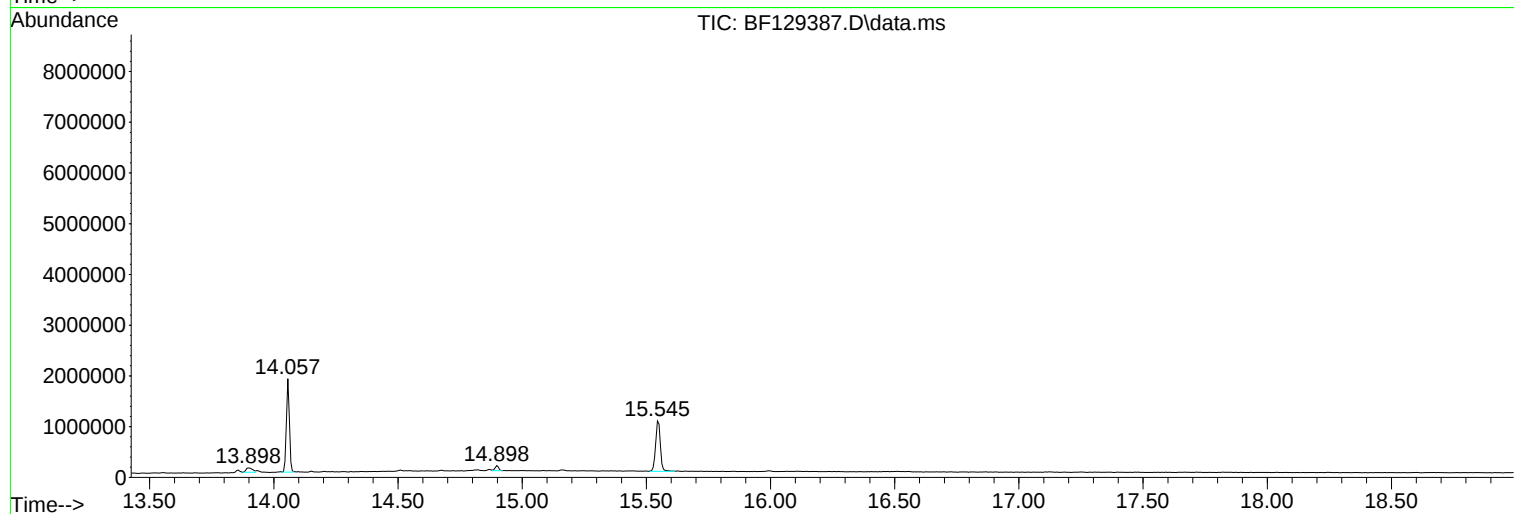
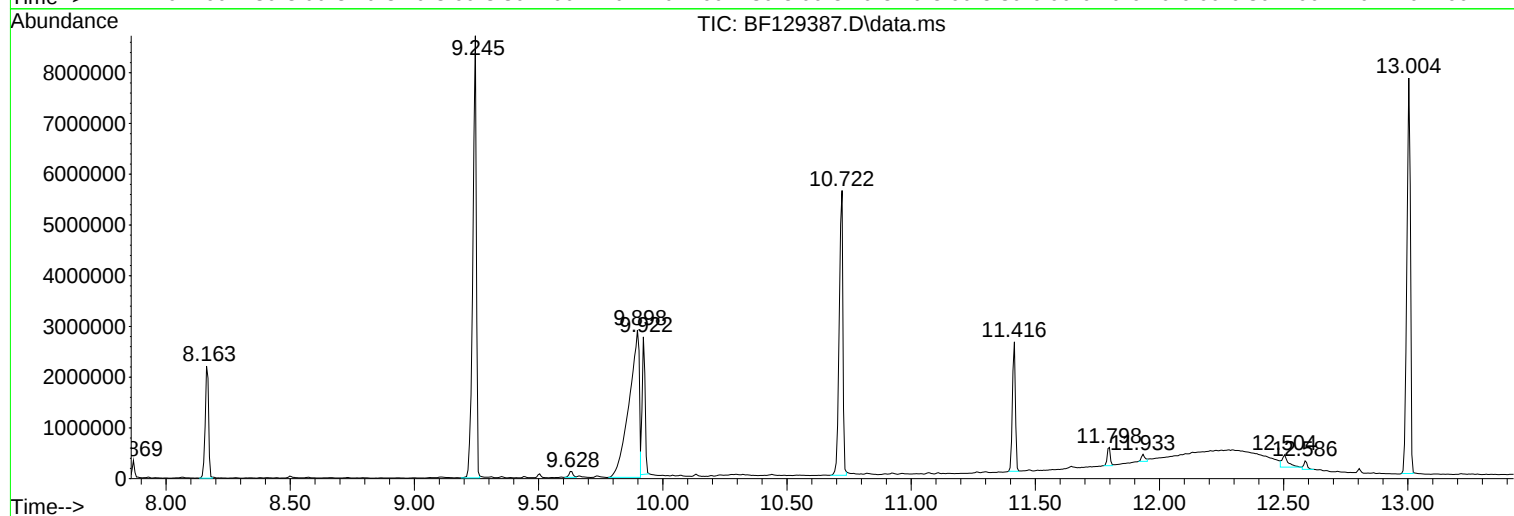
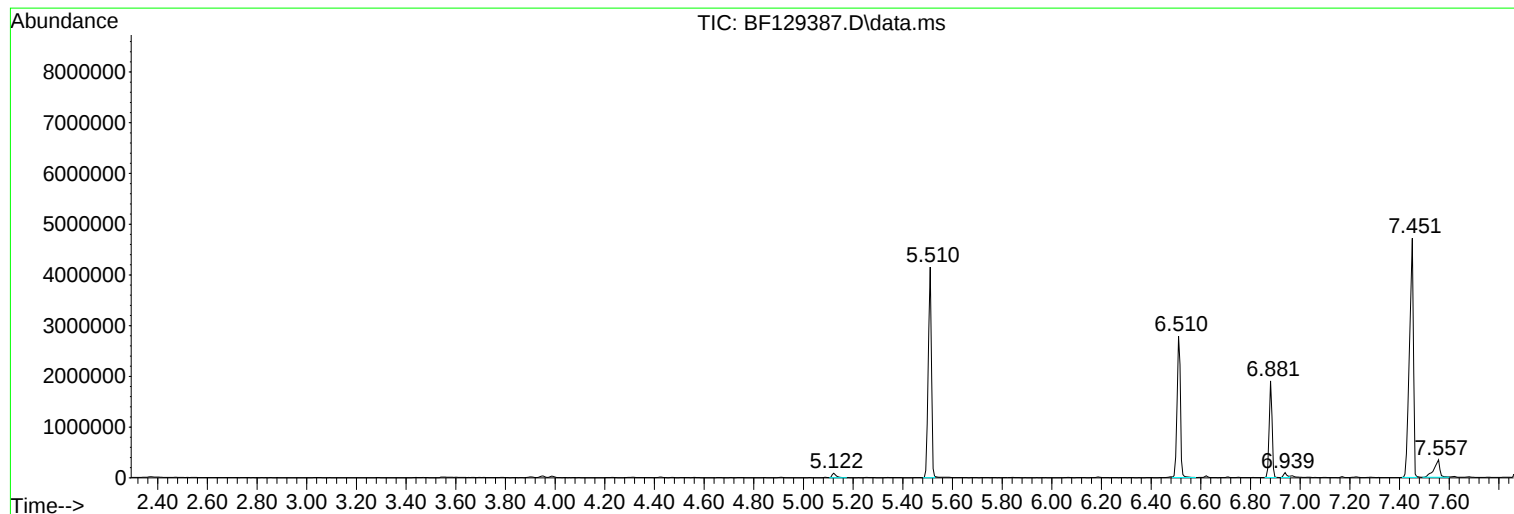
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ALS Vial : 12 Sample Multiplier: 1

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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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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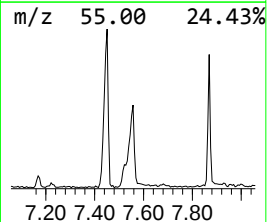
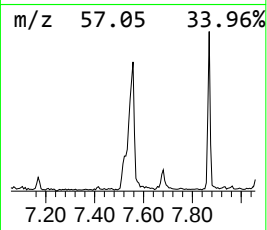
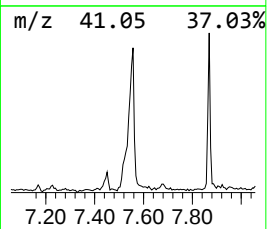
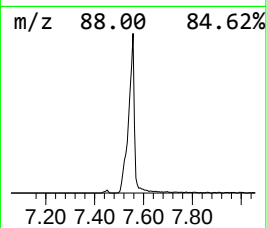
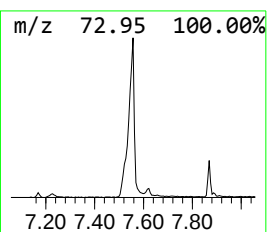
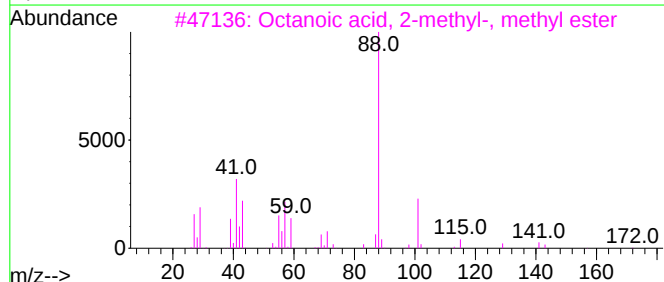
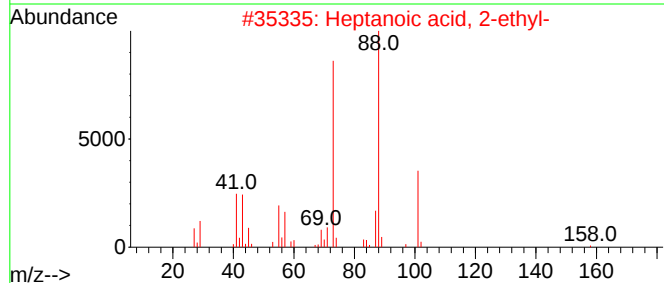
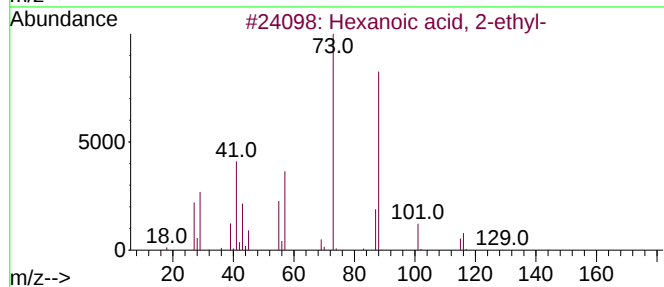
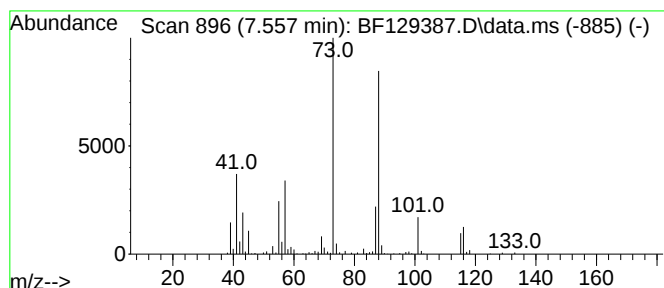
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.557	5.37 ng	570799	Naphthalene-d8	8.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2			Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
3			Octanoic acid, 2-methyl-, methyl...	172	C10H20O2	002177-86-8	47
4			1,3,6-Trioxocane	118	C5H10O3	001779-19-7	47
5			1,4-Dioxane	88	C4H8O2	000123-91-1	43



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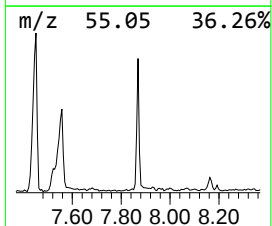
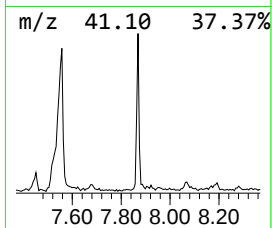
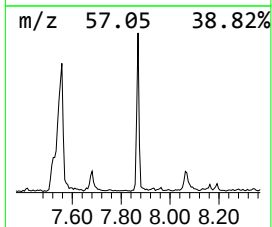
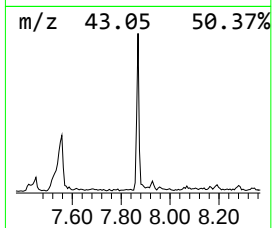
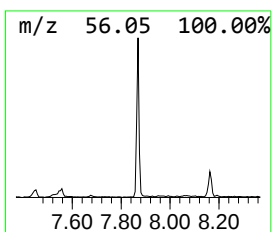
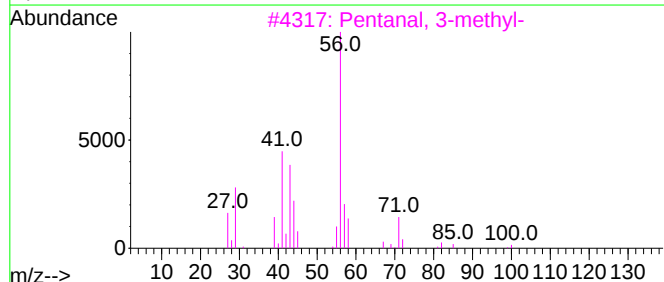
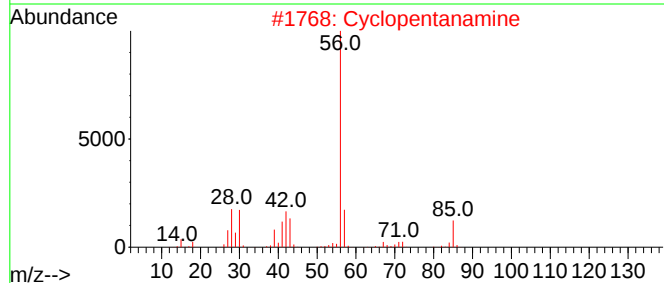
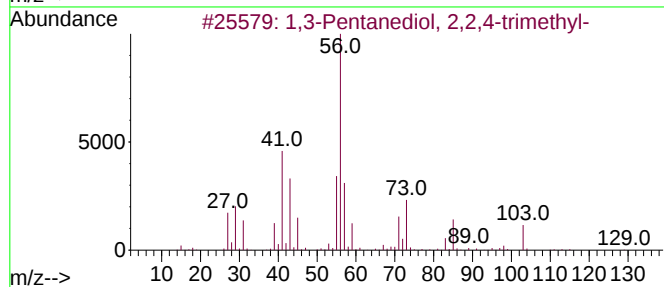
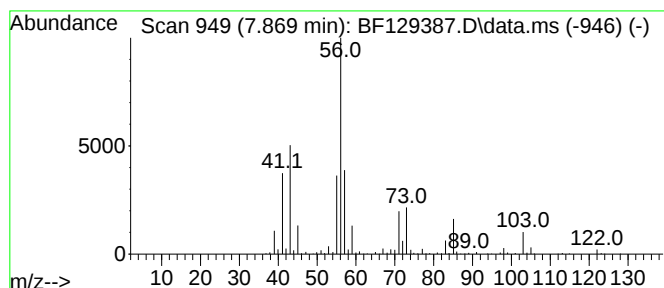
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 1,3-Pentanediol, 2,2,4-trim... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.869	2.21 ng	235028	Naphthalene-d8	8.163

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	86	
2	Cyclopentanamine	85	C5H11N	001003-03-8	37	
3	Pentanal, 3-methyl-	100	C6H12O	015877-57-3	36	
4	1,3-Hexanediol, 2-ethyl- (isomer 2)	146	C8H18O2	1000484-18-1	23	
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	23	



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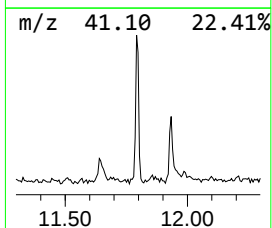
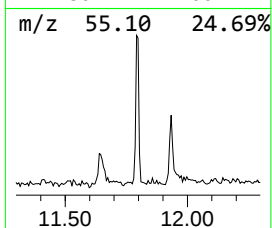
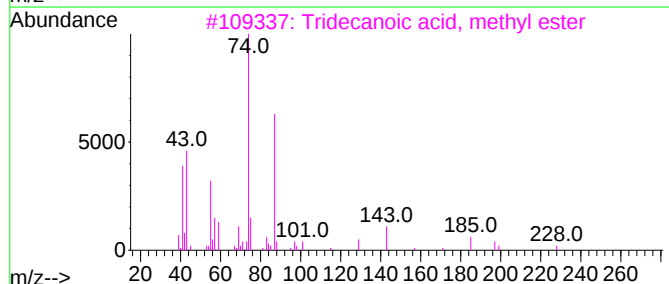
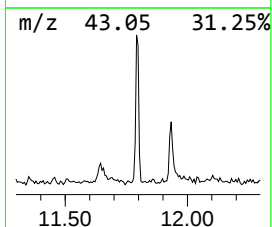
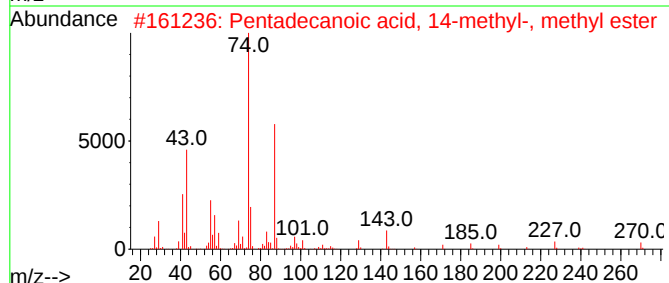
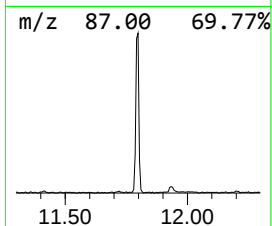
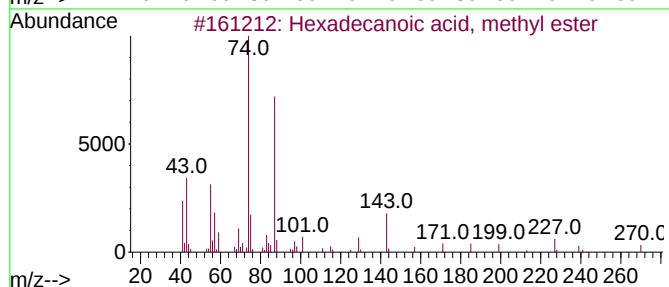
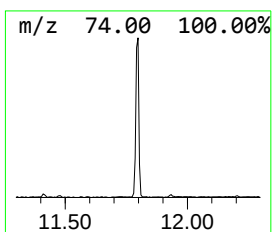
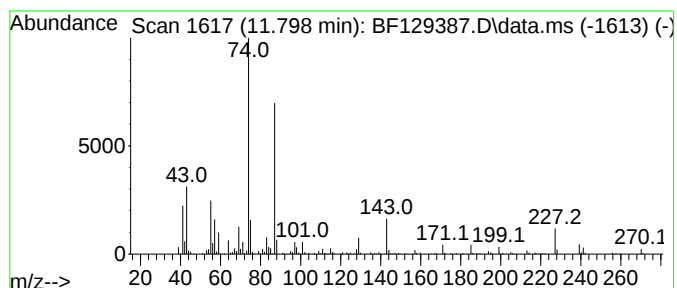
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.798	2.90 ng	314772	Phenanthrene-d10	11.416	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
5	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	87



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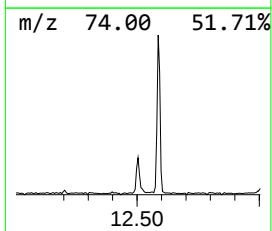
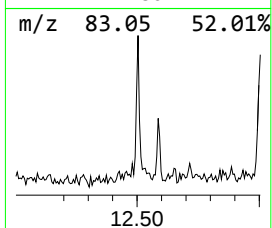
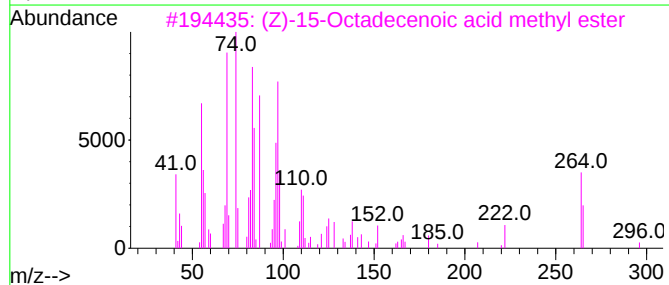
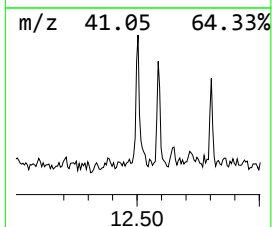
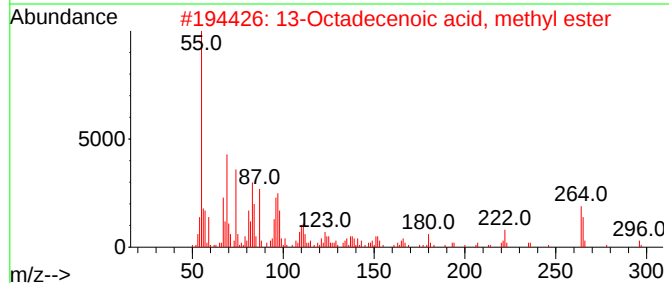
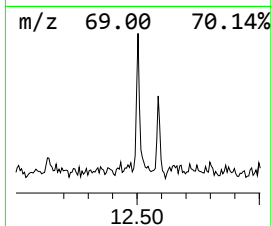
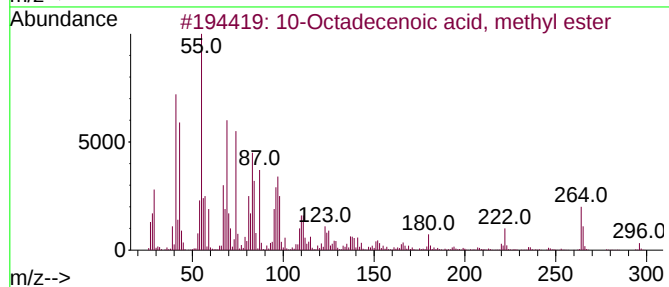
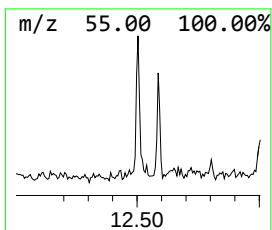
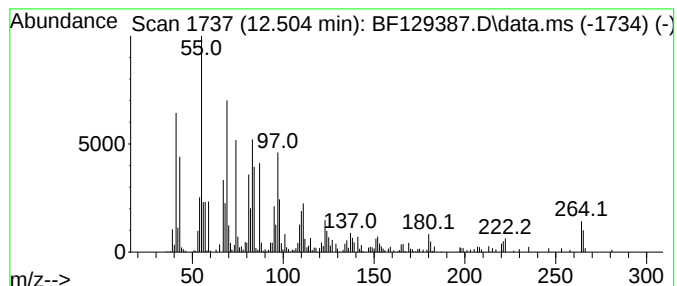
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Peak Number 4 10-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.504	3.61 ng	392138	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	87
2			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	87
3			(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	86
4			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	74
5			15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	64



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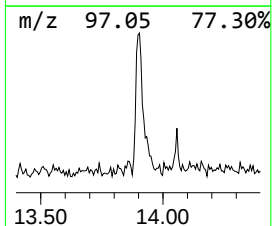
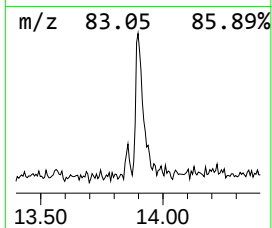
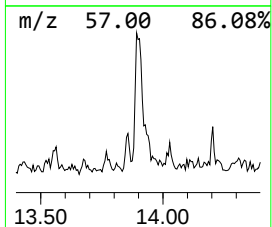
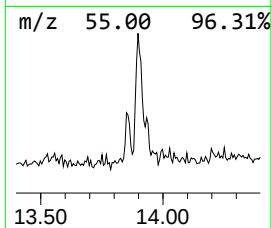
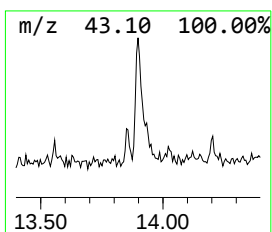
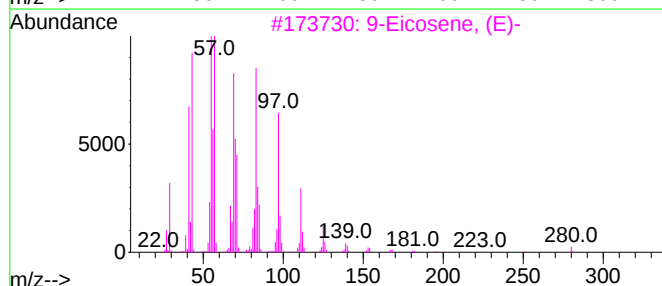
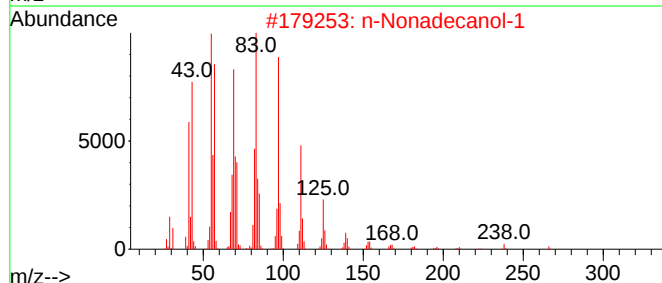
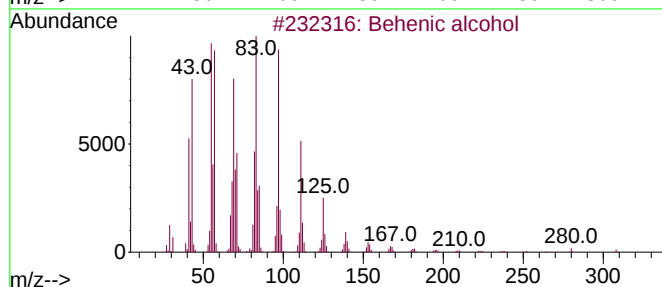
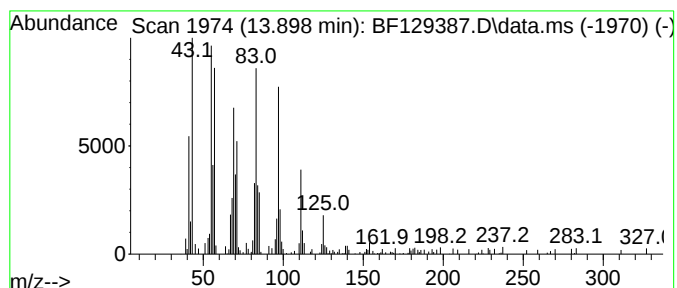
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Peak Number 5 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	2.12 ng	163743	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	94
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	93
3			9-Eicosene, (E)-	280	C20H40	074685-29-3	92
4			Cyclotridecane	182	C13H26	000295-02-3	91
5			1-Heneicosanol	312	C21H44O	015594-90-8	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanoic acid, ...	7.557	5.4	ng	570799	2	8.163	2126860	20.0
1,3-Pentanediol...	7.869	2.2	ng	235028	2	8.163	2126860	20.0
Hexadecanoic ac...	11.798	2.9	ng	314772	4	11.416	2170780	20.0
10-Octadecenoic...	12.504	3.6	ng	392138	4	11.416	2170780	20.0
Behenic alcohol	13.898	2.1	ng	163743	5	14.057	1547390	20.0