

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031824\
 Data File : BF137623.D
 Acq On : 18 Mar 2024 11:06
 Operator : CG\JU
 Sample : PB159612BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB159612BL

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-BF022924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137623.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.946	481	486	501	rBV	163321	262787	4.30%	0.655%
2	5.346	550	554	578	rBV	4695262	5605805	91.77%	13.973%
3	6.369	723	728	731	rBV	4932472	5368974	87.89%	13.383%
4	6.722	785	788	804	rBV	1239944	1236721	20.25%	3.083%
5	7.293	880	885	888	rBV	3453159	3453966	56.54%	8.609%
6	8.004	1002	1006	1025	rBV	1735638	1670504	27.35%	4.164%
7	9.087	1184	1190	1193	rBV	6231568	6108746	100.00%	15.227%
8	9.757	1300	1304	1316	rBV	2187910	1853310	30.34%	4.620%
9	10.545	1434	1438	1456	rBV	3420114	3473011	56.85%	8.657%
10	11.239	1553	1556	1578	rBV	1999397	1785541	29.23%	4.451%
11	12.651	1793	1796	1803	rBV	184674	150067	2.46%	0.374%
12	12.827	1822	1826	1830	rBV	5759298	6002212	98.26%	14.961%
13	13.357	1912	1916	1921	rBV2	138588	134455	2.20%	0.335%
14	13.874	2000	2004	2016	rBV	1384483	1294976	21.20%	3.228%
15	14.651	2132	2136	2141	rBV	73768	72263	1.18%	0.180%
16	14.968	2187	2190	2195	rVB	83181	88507	1.45%	0.221%
17	15.298	2241	2246	2250	rBV	784264	1003653	16.43%	2.502%
18	15.327	2250	2251	2260	rVB	125231	147675	2.42%	0.368%
19	15.739	2316	2321	2331	rBV	83703	132558	2.17%	0.330%
20	16.221	2398	2403	2410	rVB2	64768	113647	1.86%	0.283%
21	16.774	2492	2497	2505	rVB3	41067	86189	1.41%	0.215%
22	17.433	2603	2609	2619	rBV2	29739	73289	1.20%	0.183%

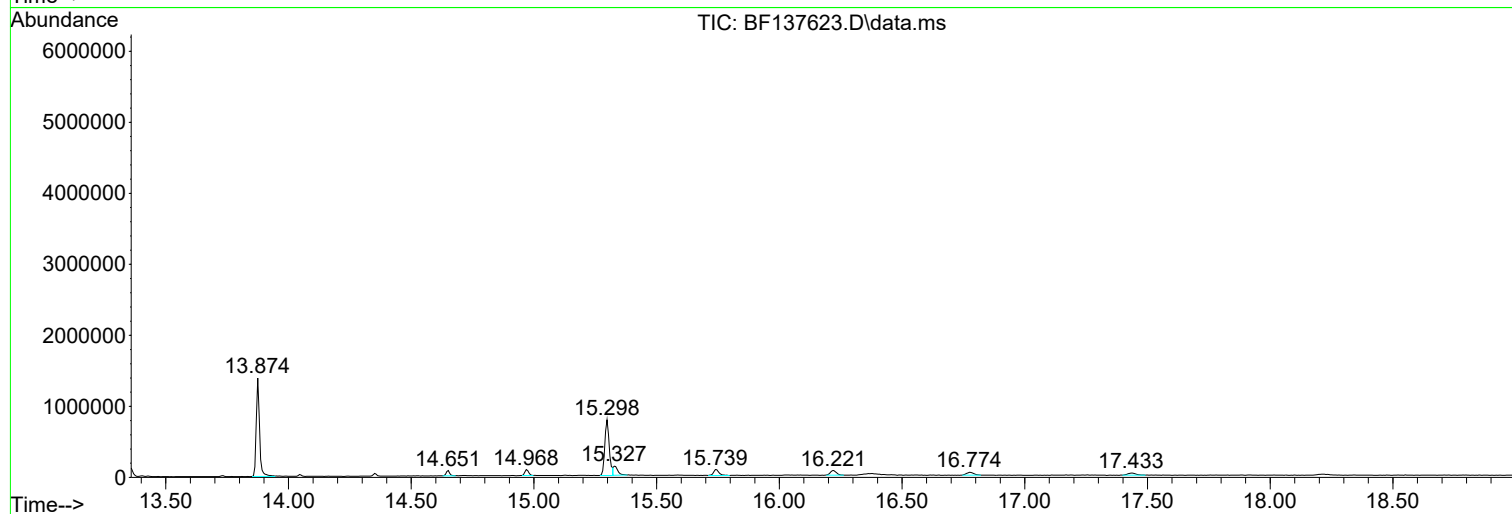
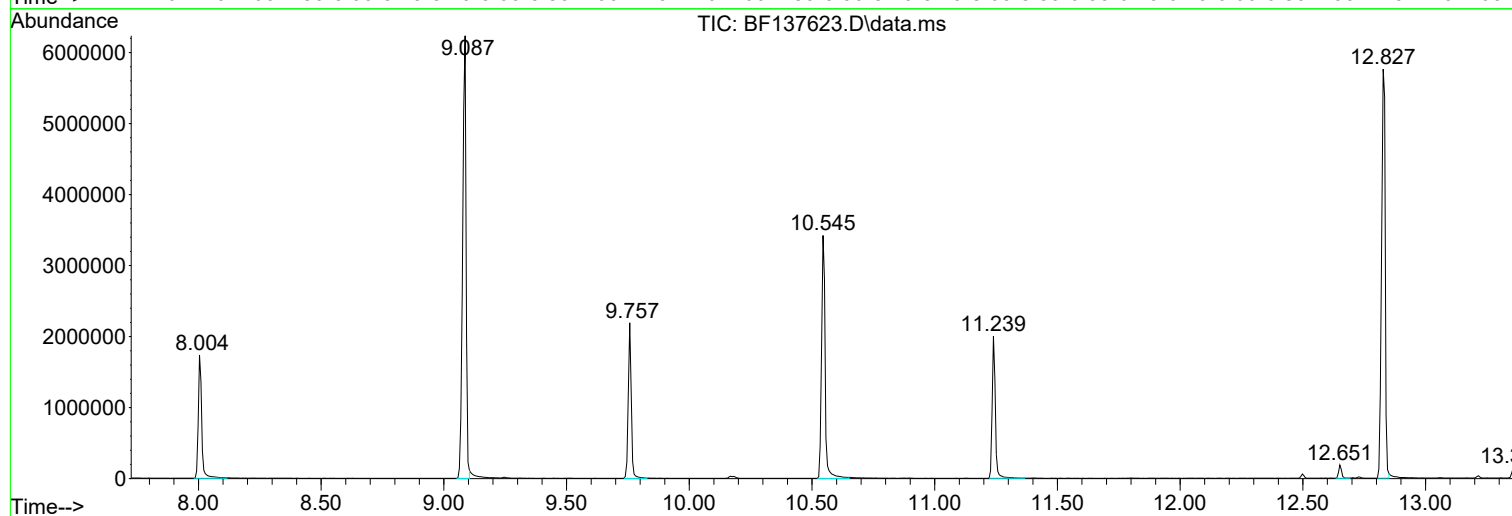
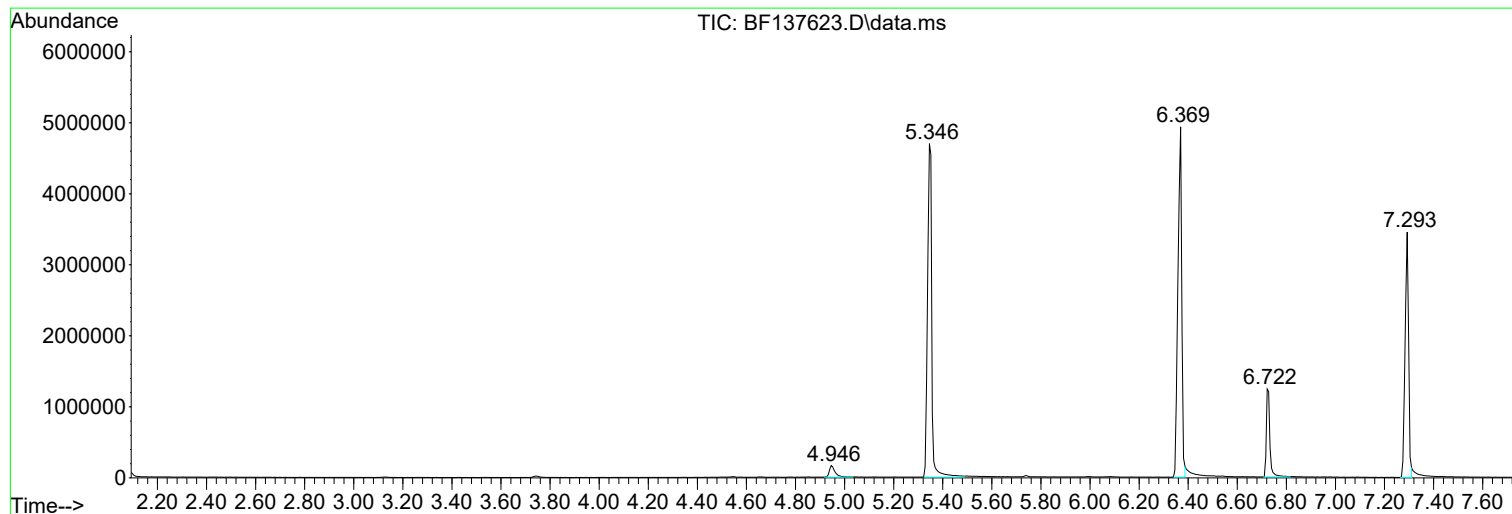
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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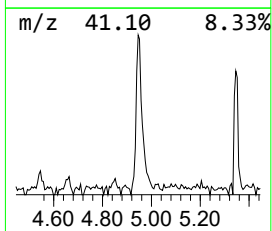
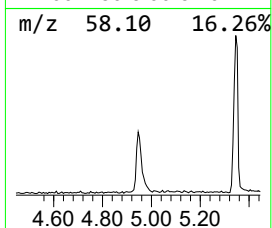
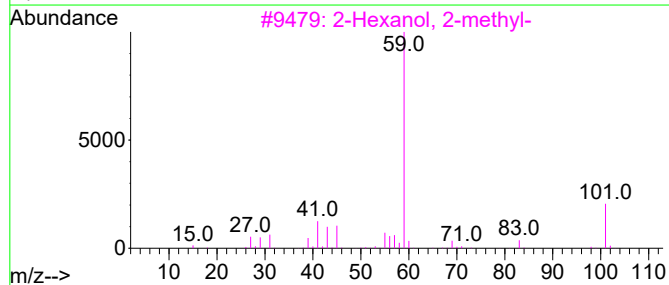
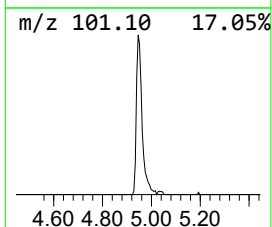
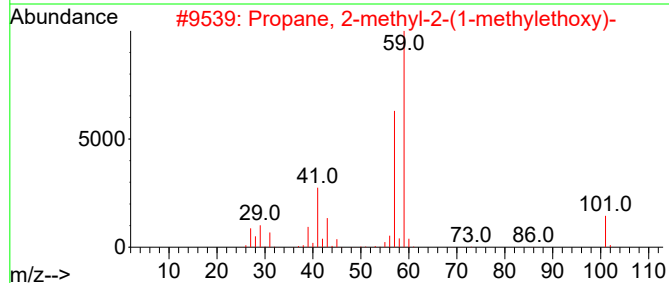
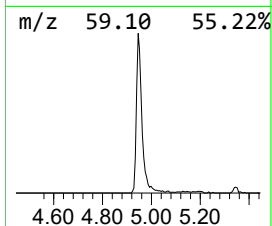
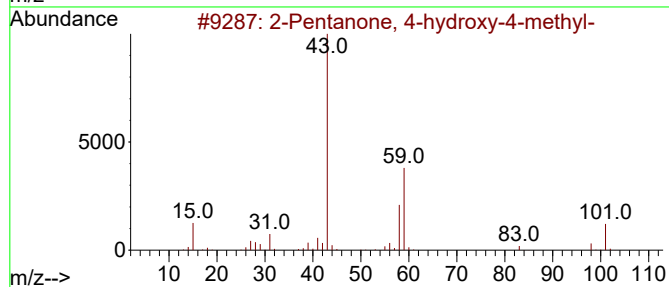
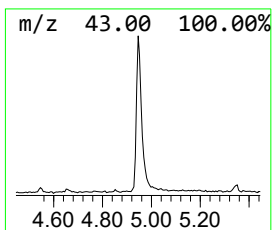
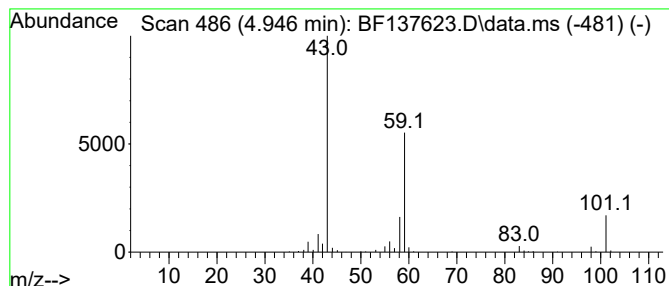
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.946	4.25 ng	262787	1,4-Dichlorobenzene-d4	6.728

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17		



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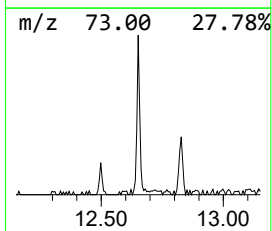
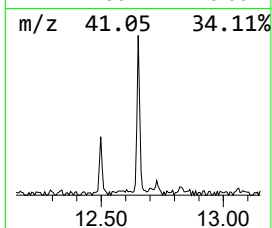
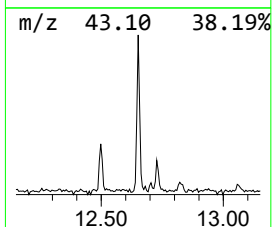
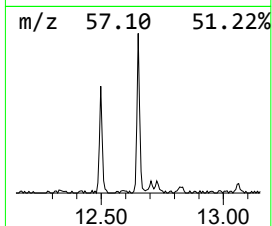
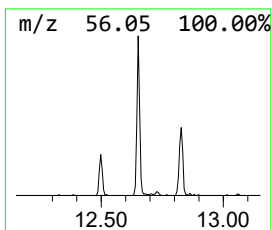
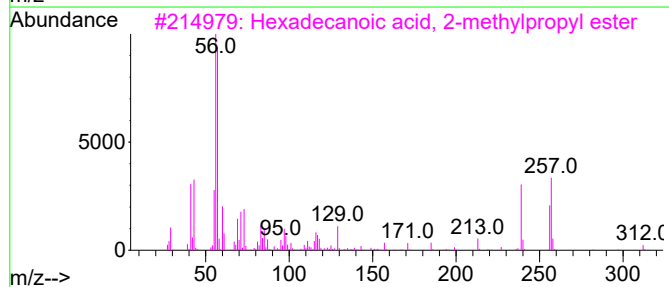
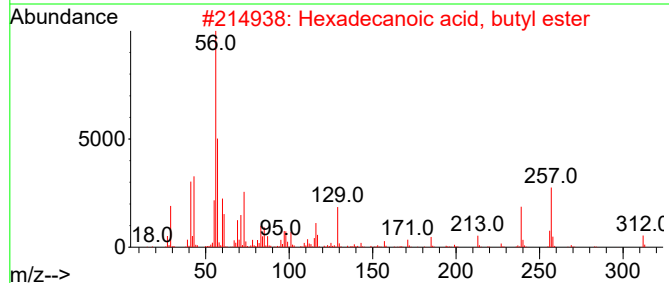
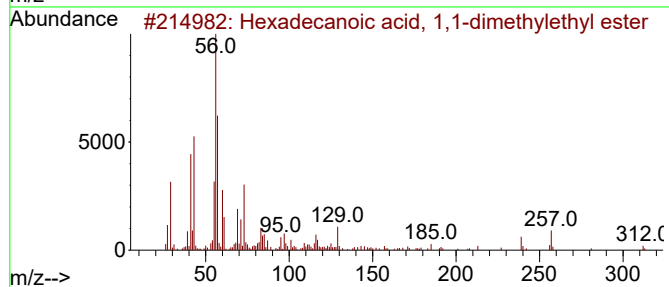
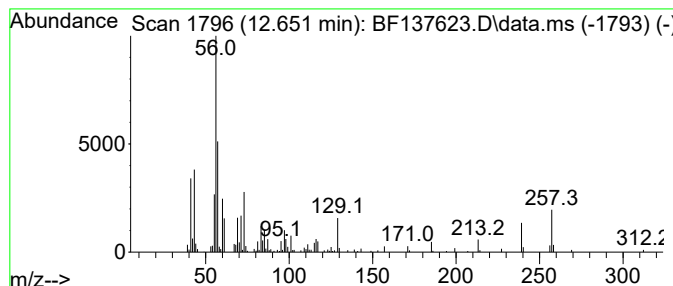
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexadecanoic acid, 1,1-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.651	2.32 ng	150067	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	87
2			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	83
3			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	45
4			Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	35
5			Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	27



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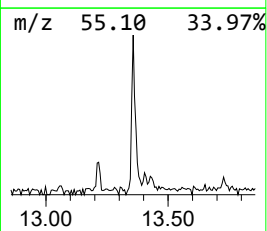
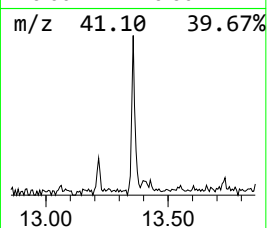
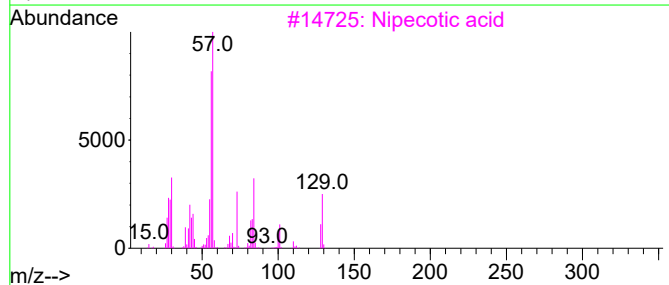
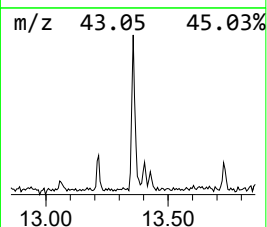
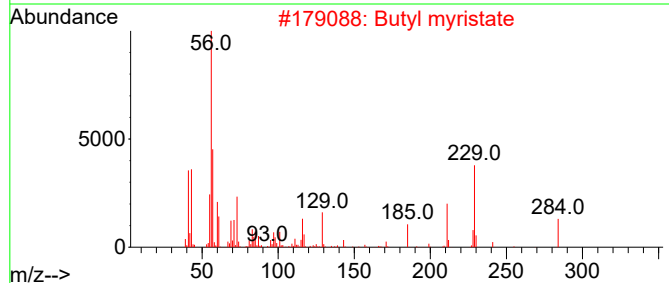
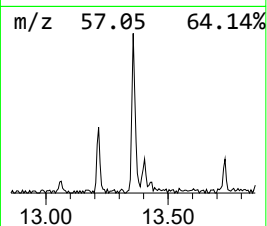
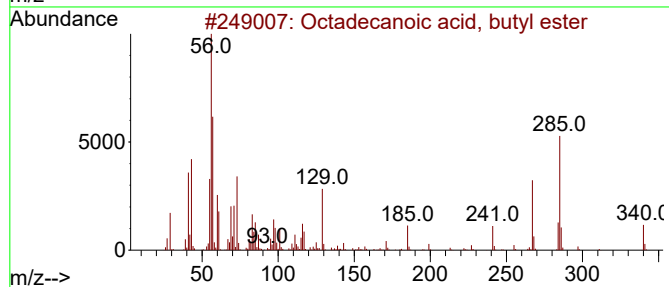
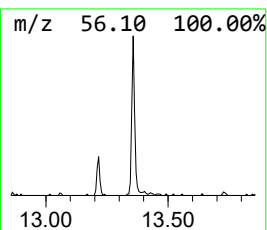
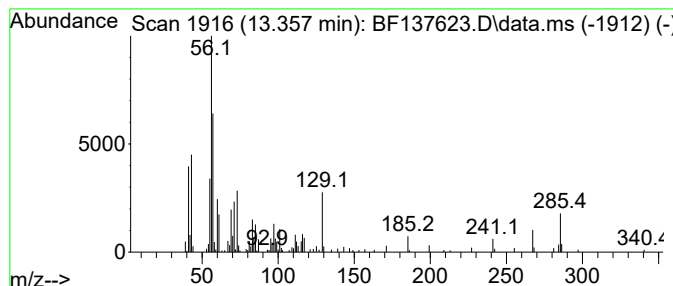
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.357	2.08 ng	134455	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	94
2			Butyl myristate	284	C18H36O2	000110-36-1	59
3			Nipecotic acid	129	C6H11NO2	000498-95-3	50
4			Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	38
5			1-Piperidinyloxy, 4-(hydroxyimin...	185	C9H17N2O2	003229-75-2	35



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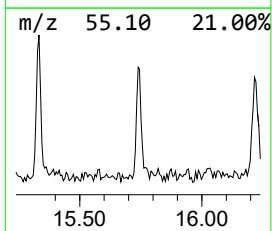
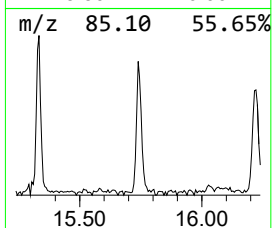
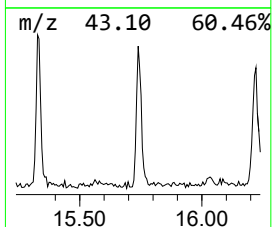
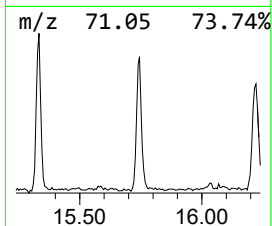
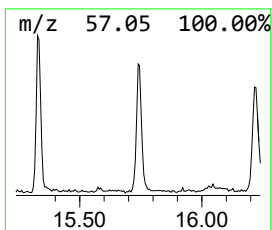
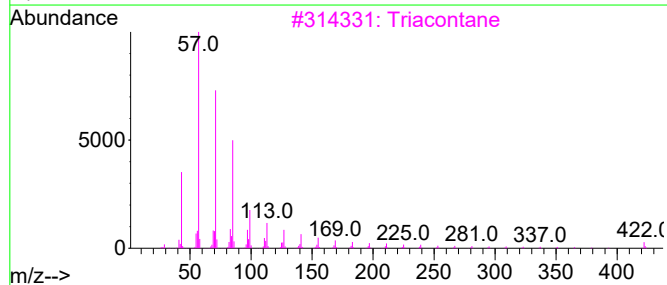
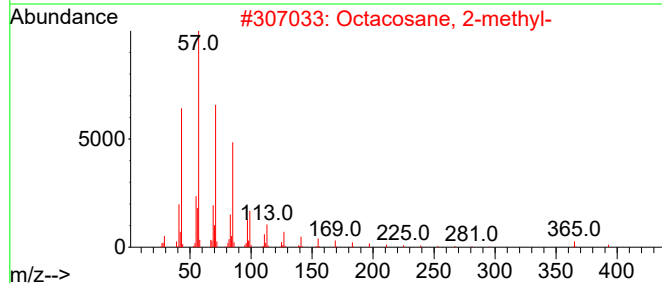
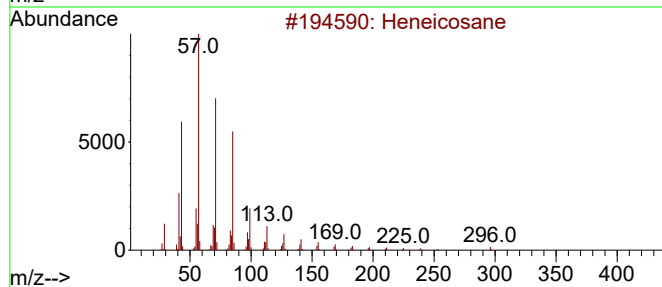
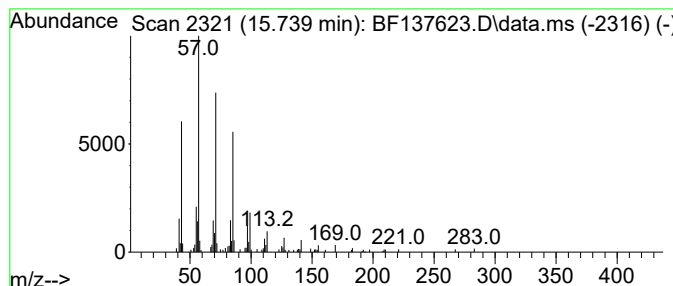
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Peak Number 4 Heneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.739	2.64 ng	132558	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Triacontane	422	C30H62	000638-68-6	91
4			Hexacosane	366	C26H54	000630-01-3	91
5			Octadecane	254	C18H38	000593-45-3	90



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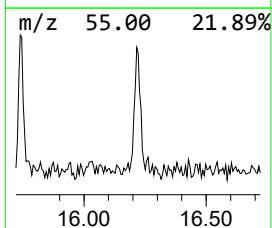
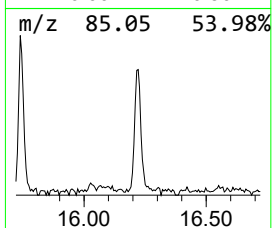
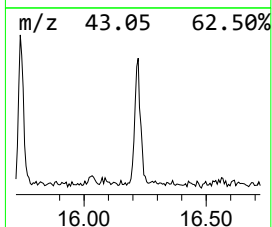
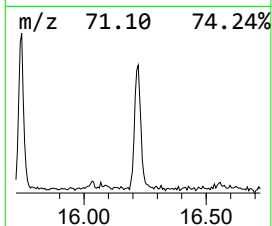
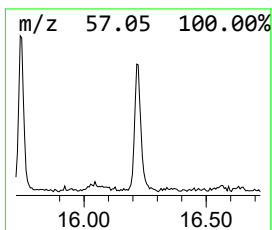
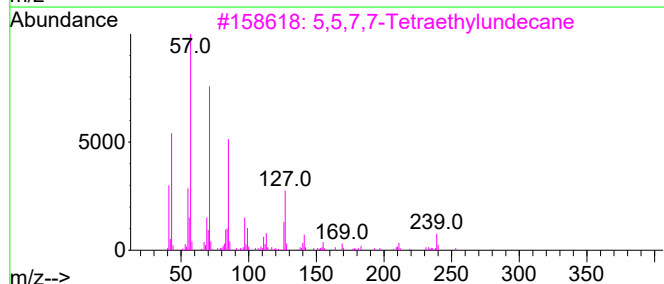
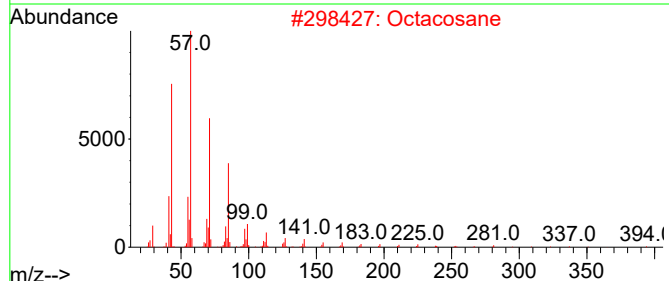
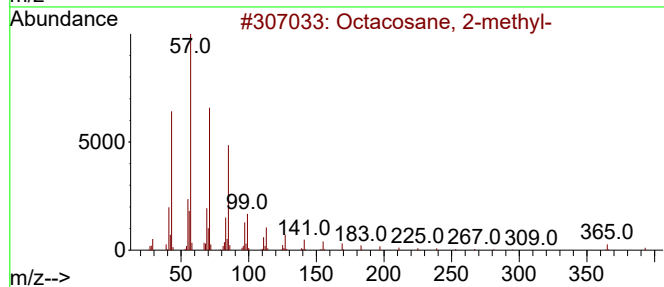
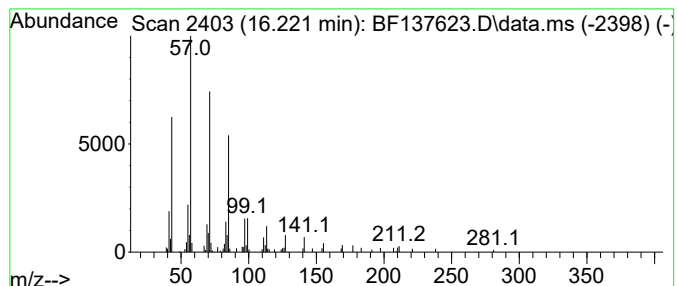
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octacosane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.221	2.26 ng	113647	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2			Octacosane	394	C28H58	000630-02-4	90
3			5,5,7,7-Tetraethylundecane	268	C19H40	1000360-42-0	90
4			Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1010115-66-1	90
5			Triacontane	422	C30H62	000638-68-6	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.946	4.3	ng	262787	1	6.728	1236720	20.0
Hexadecanoic ac...	12.651	2.3	ng	150067	5	13.874	1294980	20.0
Octadecanoic ac...	13.357	2.1	ng	134455	5	13.874	1294980	20.0
Heneicosane	15.739	2.6	ng	132558	6	15.298	1003650	20.0
Octacosane, 2-m...	16.221	2.3	ng	113647	6	15.298	1003650	20.0