

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
 Data File : BF123595.D
 Acq On : 16 Apr 2021 16:48
 Operator : JU/CG
 Sample : PB135774BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB135774BL

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-BF041521.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123595.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	11	18	23	rVB	253009	332908	3.73%	0.563%
2	5.492	574	579	582	rBV	8005035	8197213	91.85%	13.858%
3	6.498	744	750	753	rBV	7507630	8156302	91.39%	13.789%
4	6.869	809	813	816	rBV	1952042	1589029	17.81%	2.686%
5	7.433	903	909	912	rBV	4875427	5523099	61.89%	9.337%
6	8.151	1026	1031	1034	rBV	2423838	2069714	23.19%	3.499%
7	9.233	1209	1215	1218	rBV	9216241	8655826	96.99%	14.633%
8	9.910	1325	1330	1334	rBV	2390981	2183826	24.47%	3.692%
9	10.704	1457	1465	1468	rBV	6436903	5858081	65.64%	9.903%
10	11.404	1580	1584	1587	rBV	2577387	2245025	25.16%	3.795%
11	11.927	1668	1673	1686	rBV2	135177	228637	2.56%	0.387%
12	12.815	1817	1824	1829	rBV	818838	642549	7.20%	1.086%
13	12.892	1835	1837	1845	rVB	148606	124633	1.40%	0.211%
14	12.998	1850	1855	1858	rBV	9162942	8924261	100.00%	15.087%
15	13.527	1941	1945	1950	rBV	530818	501660	5.62%	0.848%
16	14.051	2027	2034	2037	rBV	1994489	1827724	20.48%	3.090%
17	14.527	2110	2115	2118	rBV	92796	91383	1.02%	0.154%
18	14.839	2163	2168	2173	rBV	106386	114745	1.29%	0.194%
19	15.186	2223	2227	2232	rVB	95217	104560	1.17%	0.177%
20	15.539	2281	2287	2291	rBV	1022139	1373841	15.39%	2.323%
21	15.574	2291	2293	2298	rVB	90069	111797	1.25%	0.189%
22	16.027	2363	2370	2378	rBV3	107756	195441	2.19%	0.330%
23	16.551	2454	2459	2466	rVB2	53806	100630	1.13%	0.170%

Sum of corrected areas: 59152884

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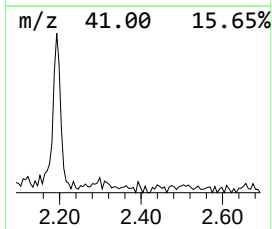
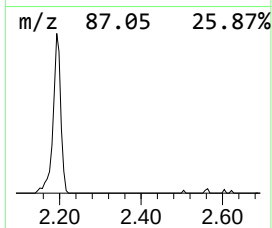
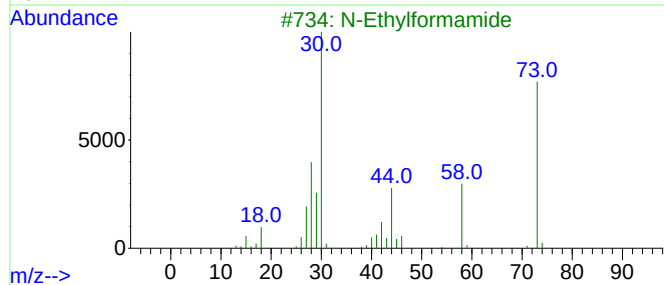
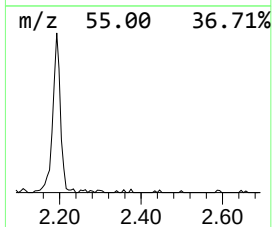
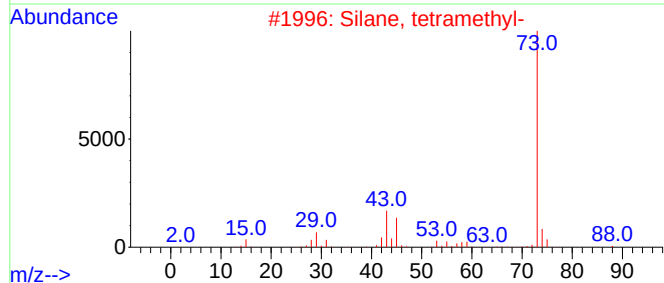
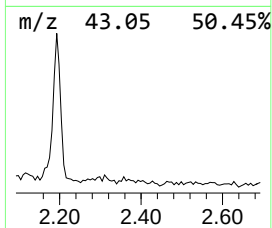
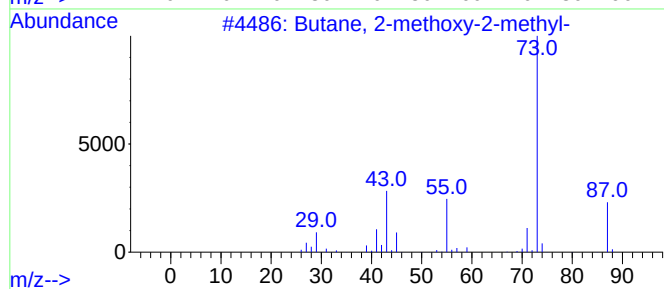
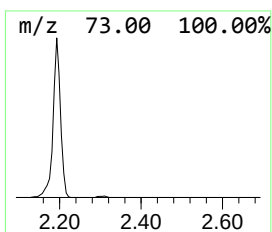
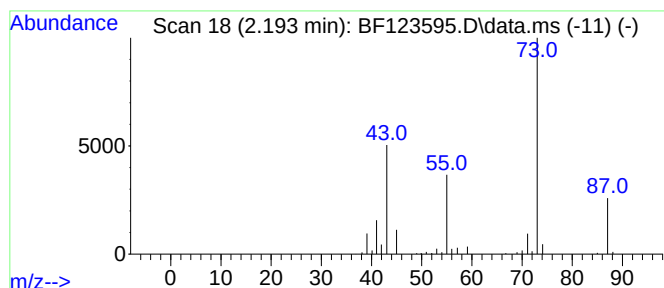
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	4.19 ng	332908	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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3			N-Ethylformamide	73	C3H7NO	000627-45-2	9
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9



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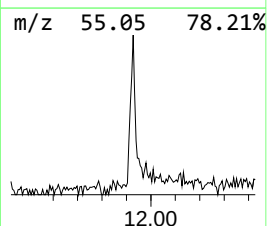
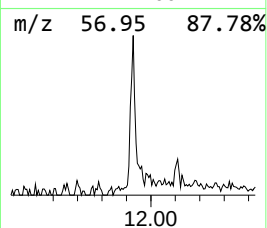
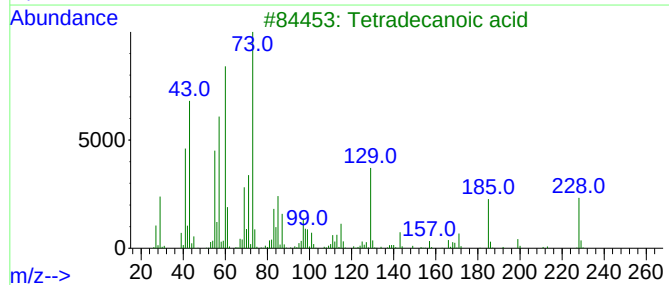
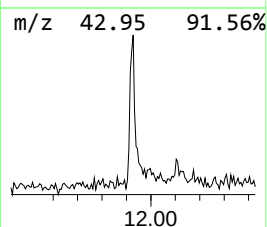
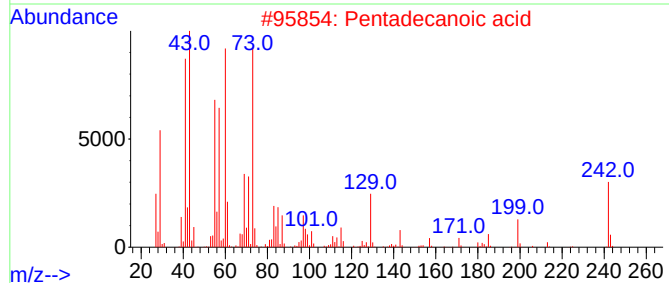
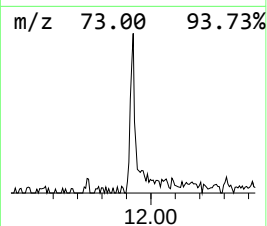
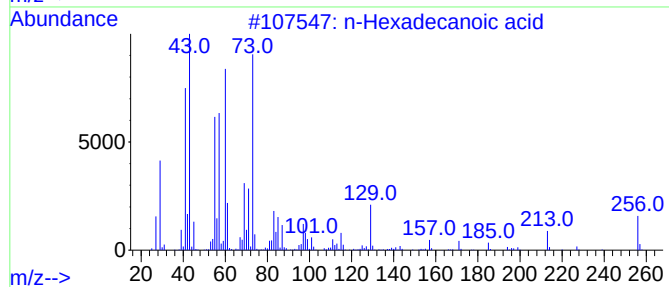
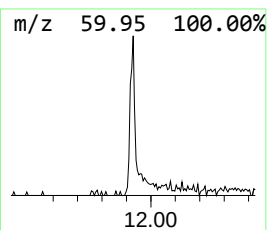
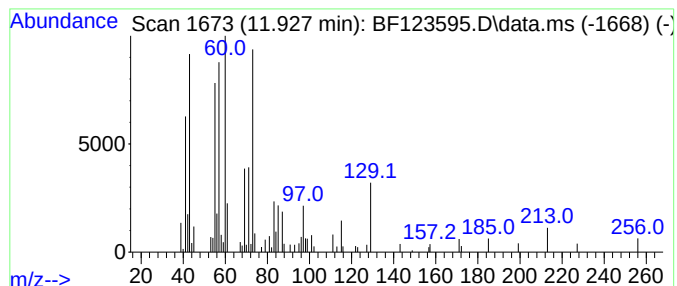
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	2.04 ng	228637	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4			Undecanoic acid	186	C11H22O2	000112-37-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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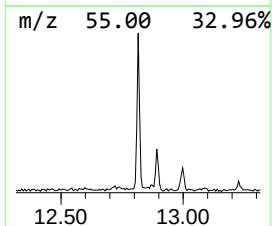
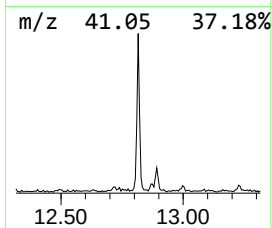
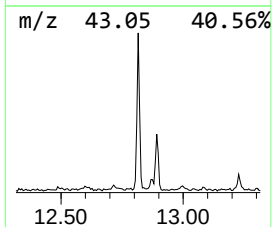
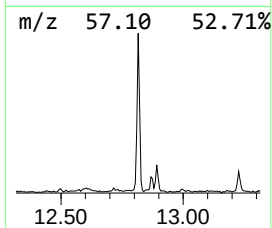
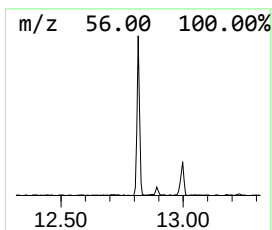
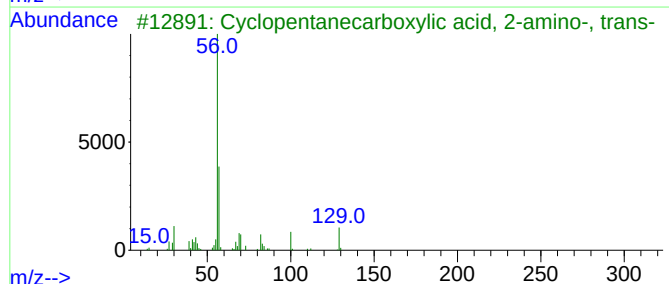
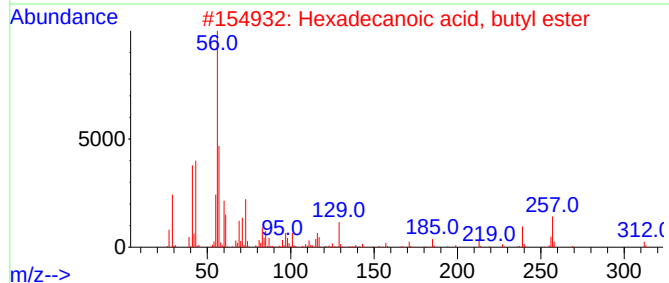
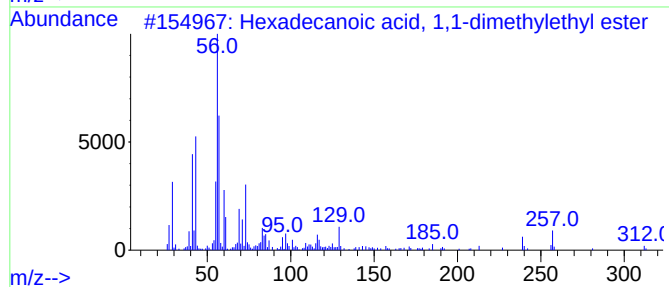
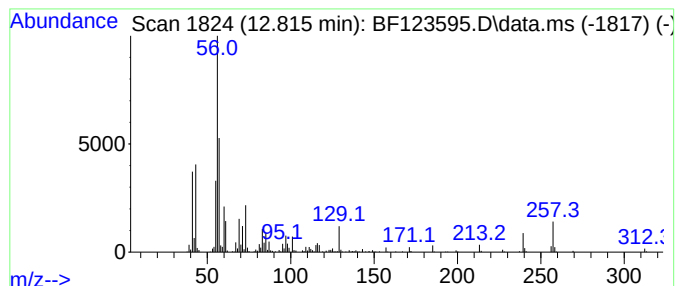
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Peak Number 3 Hexadecanoic acid, 1,1-dime... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.816	7.03 ng	642549	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	97
2			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	96
3			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	46
4			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
5			Cycloheptylamine	113	C7H15N	005452-35-7	38



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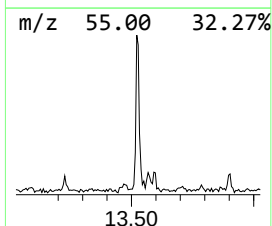
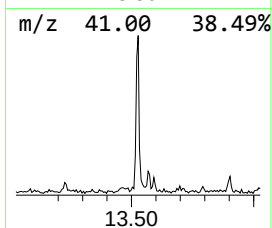
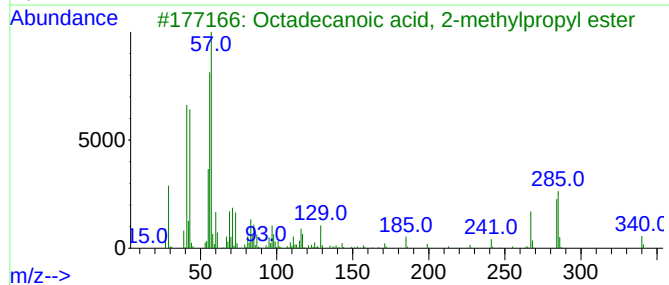
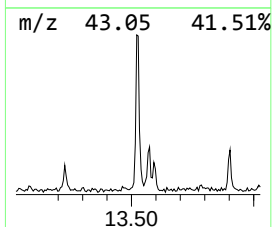
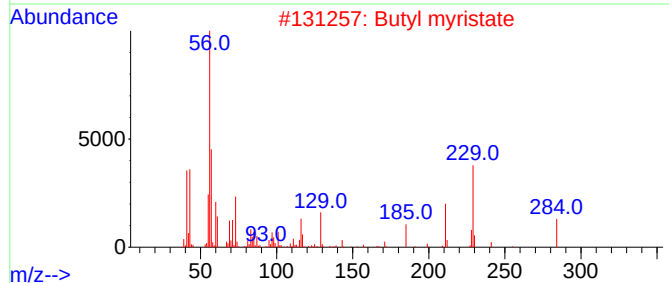
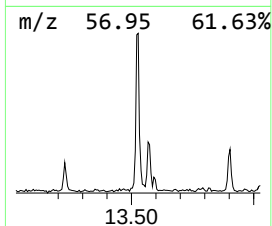
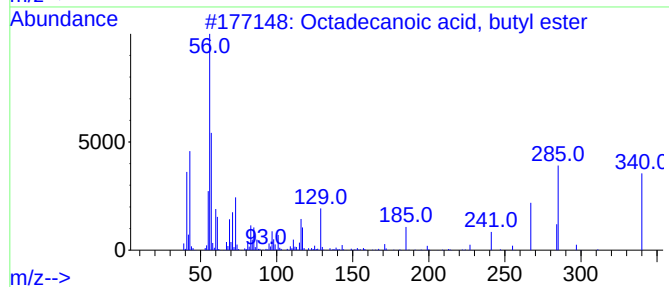
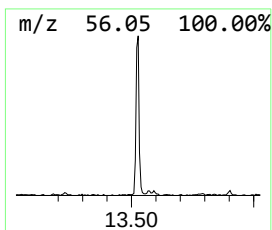
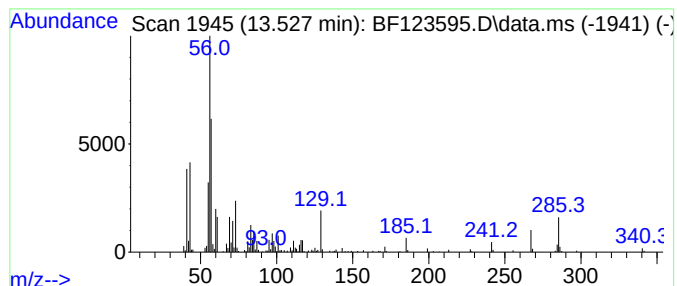
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Peak Number 4 Octadecanoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.527	5.49 ng	501660	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	96
2			Butyl myristate	284	C18H36O2	000110-36-1	80
3			Octadecanoic acid, 2-methylpropyl...	340	C22H44O2	000646-13-9	35
4			1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27
5			1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27



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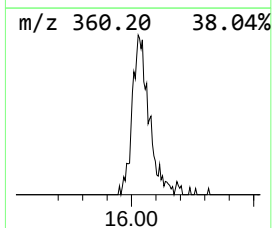
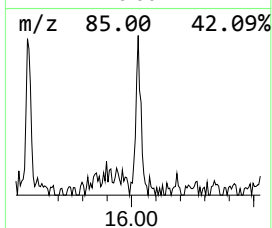
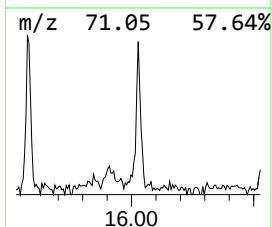
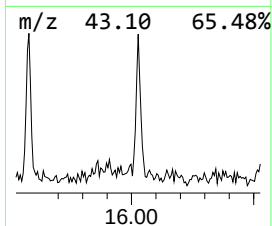
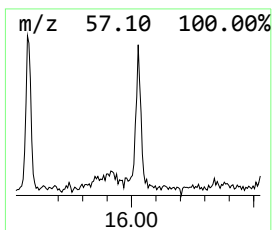
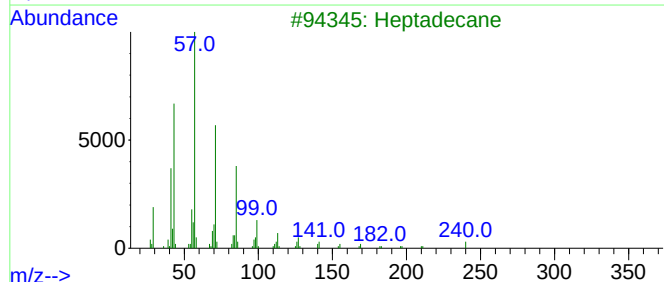
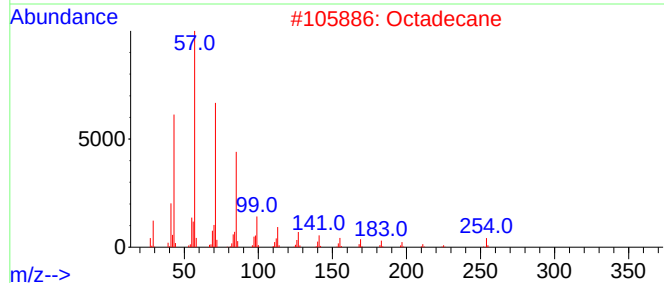
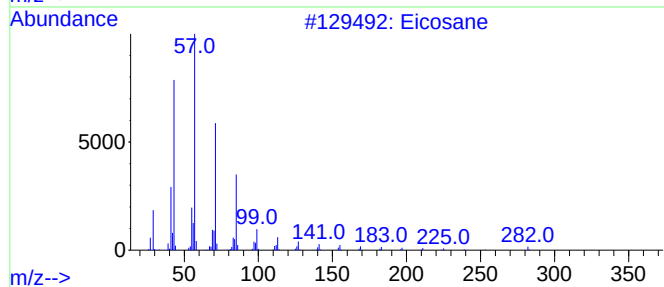
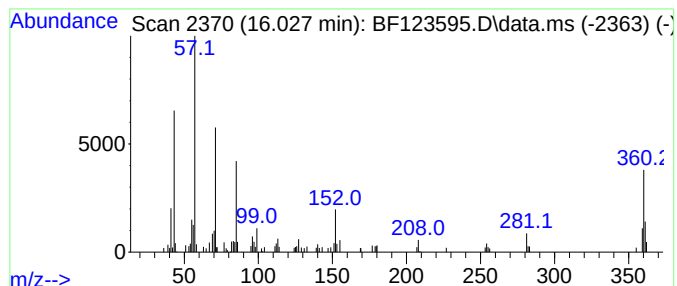
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Peak Number 5 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.027	2.85 ng	195441	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	89
2			Octadecane	254	C18H38	000593-45-3	64
3			Heptadecane	240	C17H36	000629-78-7	43
4			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	43
5			Eicosane, 10-methyl-	296	C21H44	054833-23-7	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.193	4.2	ng	332908	1	6.869	1589030	20.0
n-Hexadecanoic ...	11.927	2.0	ng	228637	4	11.404	2245030	20.0
Hexadecanoic ac...	12.816	7.0	ng	642549	5	14.051	1827720	20.0
Octadecanoic ac...	13.527	5.5	ng	501660	5	14.051	1827720	20.0
Eicosane	16.027	2.9	ng	195441	6	15.539	1373840	20.0