

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022422\
 Data File : BF127059.D
 Acq On : 24 Feb 2022 16:08
 Operator : CG\JU
 Sample : N1632-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20220094-BERKELEY-6-ELUTRIATE

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-BF021622.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127059.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.522	546	550	553	rBV	1148370	945110	36.76%	6.268%
2	6.528	717	721	729	rVB	802476	764132	29.72%	5.068%
3	6.904	781	785	788	rVB	566113	420876	16.37%	2.791%
4	7.469	876	881	884	rBV	1575375	1400903	54.49%	9.291%
5	8.081	982	985	997	rBV	40118	51862	2.02%	0.344%
6	8.187	999	1003	1007	rBV	704435	571499	22.23%	3.790%
7	9.263	1180	1186	1189	rBV	3053327	2571040	100.00%	17.052%
8	9.757	1266	1270	1284	rBV8	30246	70762	2.75%	0.469%
9	9.945	1299	1302	1306	rVB	794239	640119	24.90%	4.246%
10	10.339	1367	1369	1371	rBV	42066	36061	1.40%	0.239%
11	10.739	1432	1437	1440	rBV	2168677	1845528	71.78%	12.240%
12	11.380	1543	1546	1550	rVB	75968	58781	2.29%	0.390%
13	11.439	1552	1556	1559	rBV	873975	671425	26.11%	4.453%
14	11.598	1579	1583	1586	rBV	2363322	1839221	71.54%	12.198%
15	11.816	1617	1620	1623	rVB2	56038	47581	1.85%	0.316%
16	11.951	1639	1643	1647	rBV	150403	125332	4.87%	0.831%
17	12.739	1773	1777	1779	rBV2	39680	35580	1.38%	0.236%
18	13.027	1821	1826	1829	rBV	2344097	1907250	74.18%	12.650%
19	13.945	1973	1982	1993	rBV4	81856	231913	9.02%	1.538%
20	14.086	2002	2006	2009	rVB	457650	432079	16.81%	2.866%
21	14.392	2055	2058	2061	rBV	81544	69776	2.71%	0.463%
22	15.586	2256	2261	2266	rBV	266268	340684	13.25%	2.260%

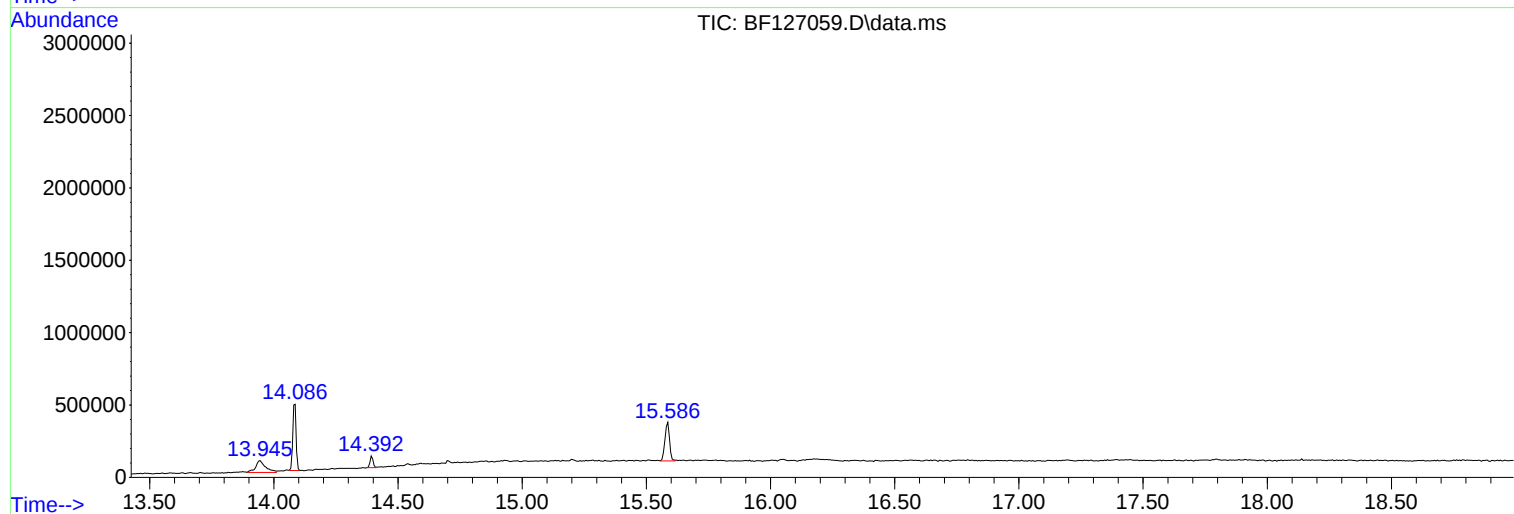
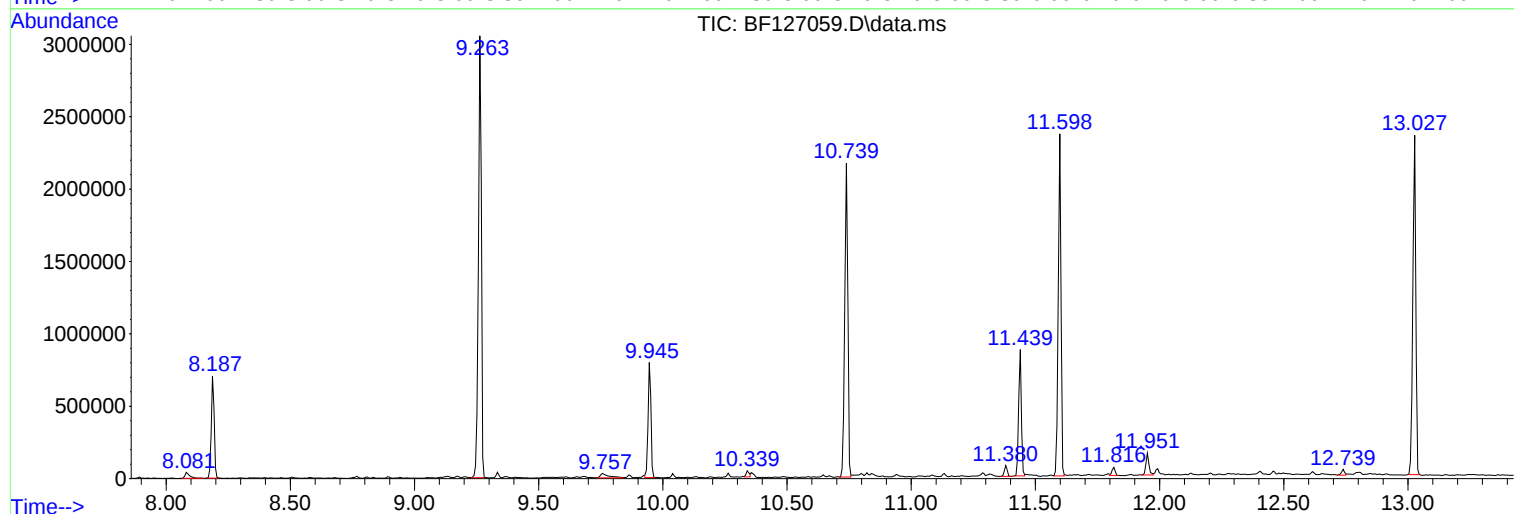
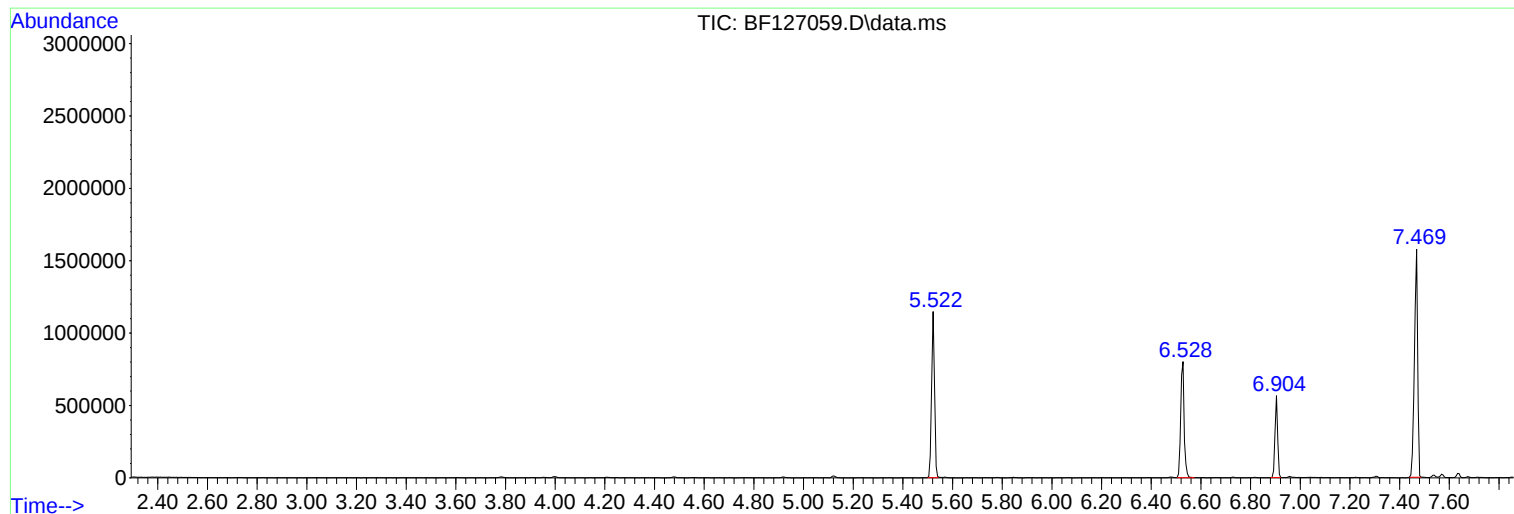
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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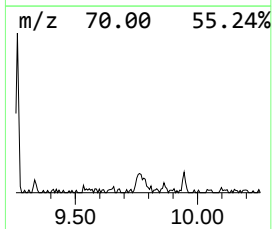
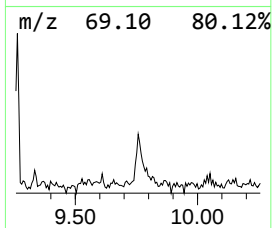
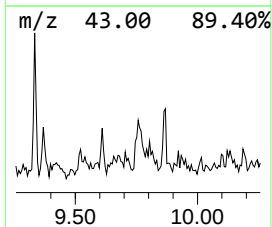
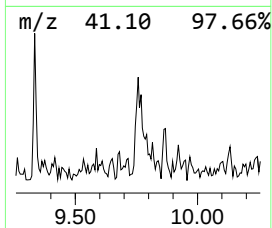
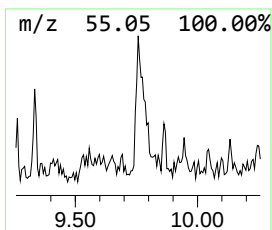
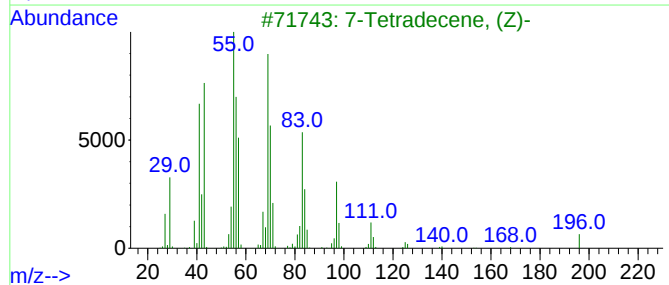
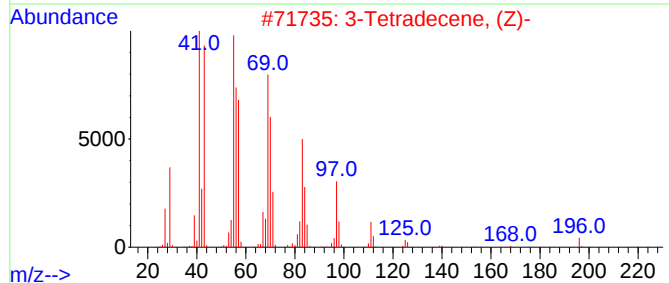
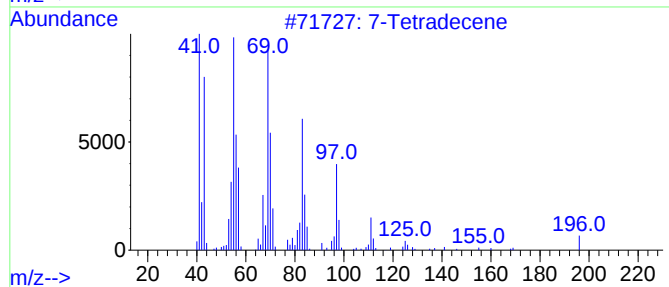
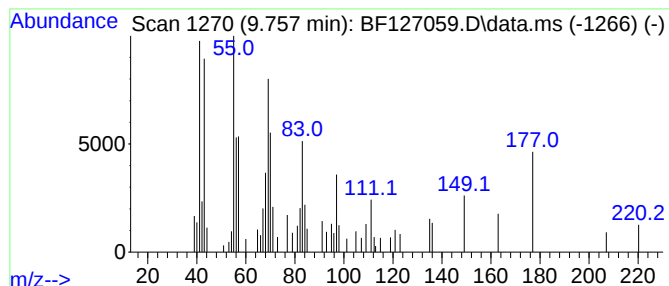
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 7-Tetradecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.757	2.21 ng	70762	Acenaphthene-d10	9.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Tetradecene	196	C14H28	010374-74-0	68
2			3-Tetradecene, (Z)-	196	C14H28	041446-67-7	68
3			7-Tetradecene, (Z)-	196	C14H28	041446-60-0	64
4			7-Tetradecene, (E)-	196	C14H28	041446-63-3	64
5			3-Tetradecene, (E)-	196	C14H28	041446-68-8	64



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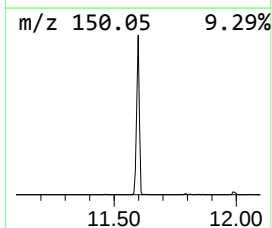
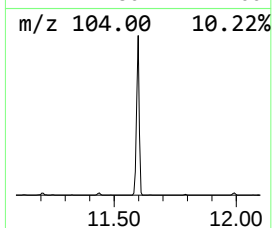
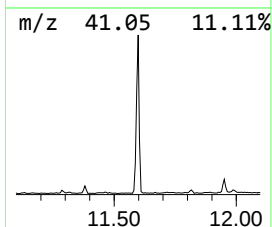
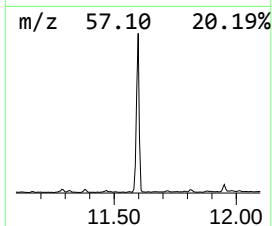
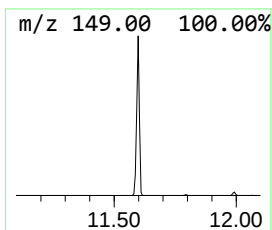
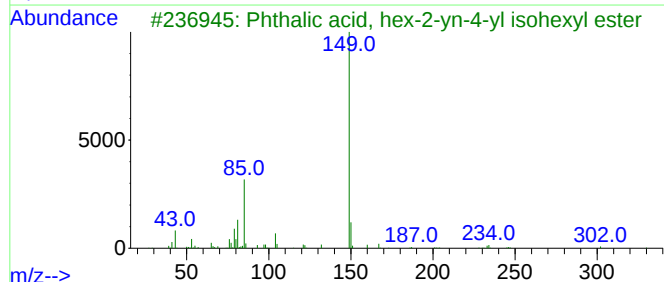
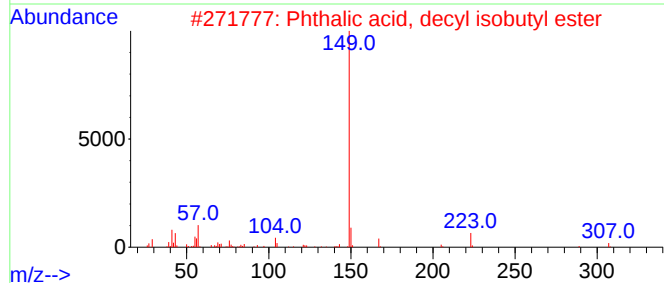
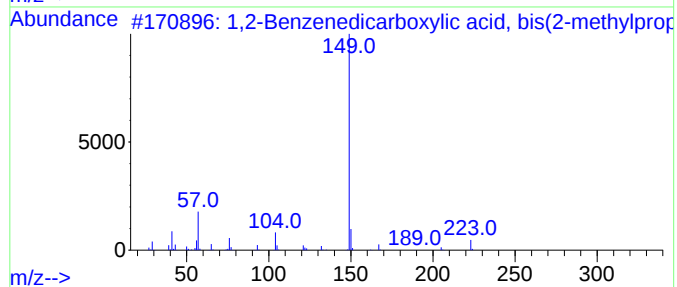
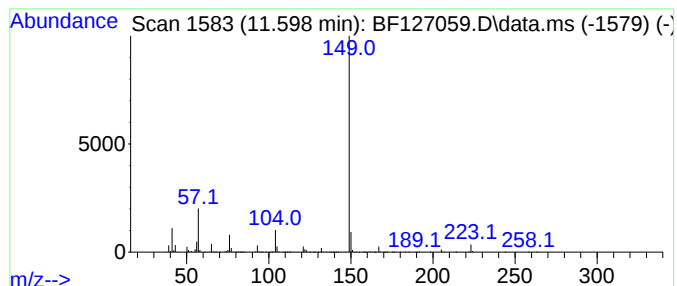
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Peak Number 2 1,2-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.598	54.79 ng	1839220	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	91
2			Phthalic acid, decyl isobutyl ester	362	C22H34O4	1000308-94-2	78
3			Phthalic acid, hex-2-yn-4-yl iso...	330	C20H26O4	1000315-20-0	78
4			Phthalic acid, 8-bromooctyl isobu...	412	C20H29BrO4	1000382-55-3	78
5			Phthalic acid, 2-ethoxyethyl pro...	280	C15H20O5	1000322-87-0	78



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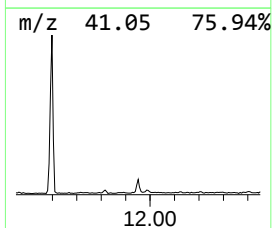
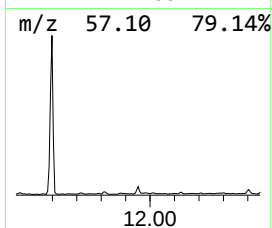
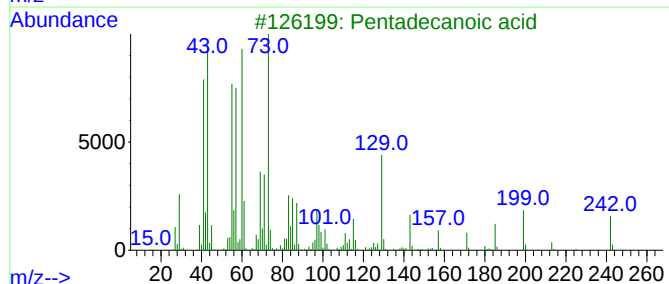
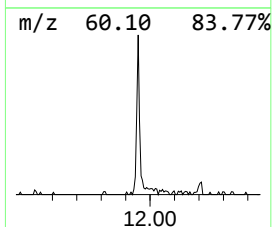
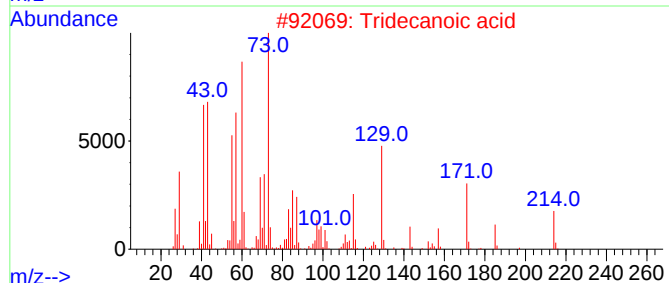
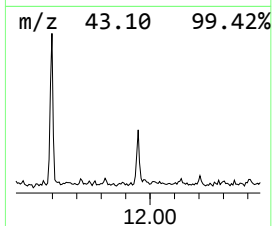
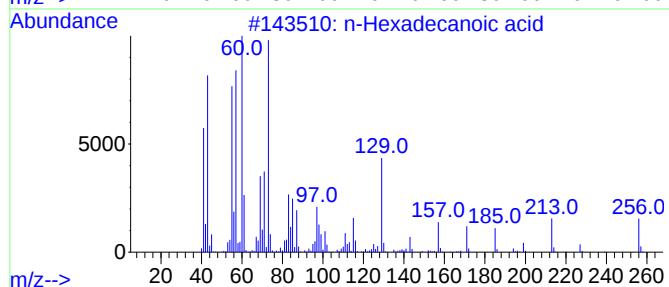
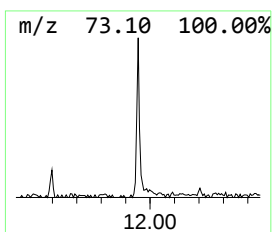
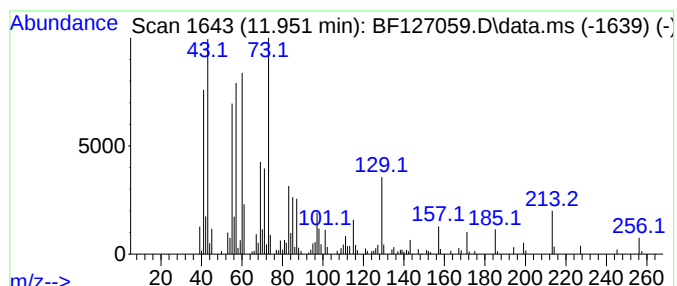
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.951	3.73 ng	125332	Phenanthrene-d10		11.439	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	98
2	Tridecanoic acid		214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	72
5	Dodecanoic acid		200	C12H24O2	000143-07-7	62



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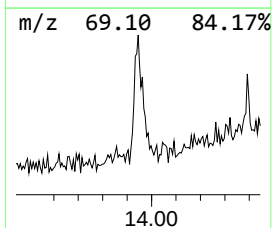
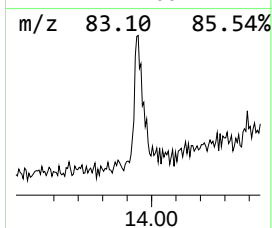
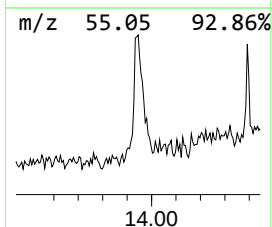
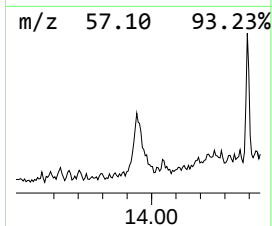
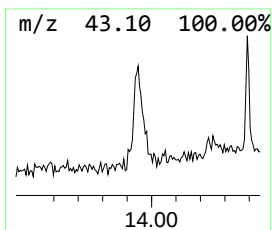
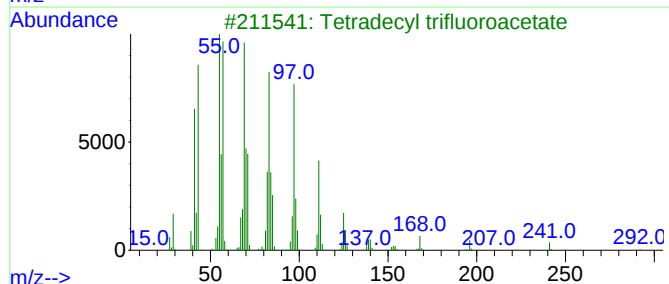
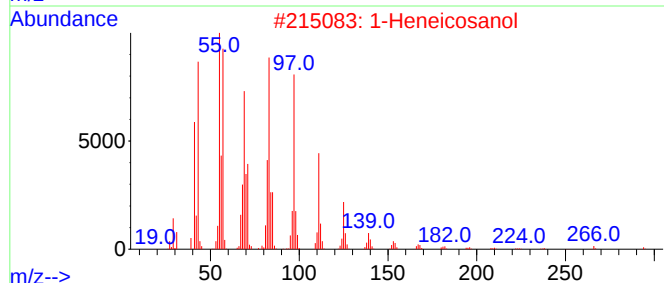
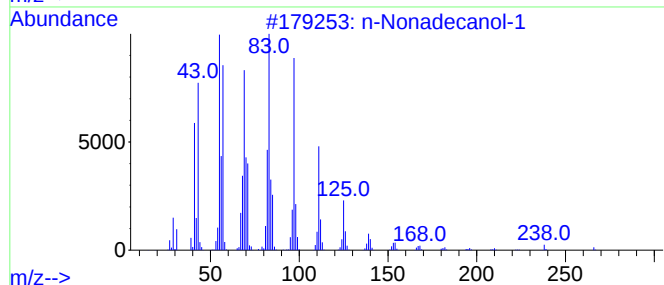
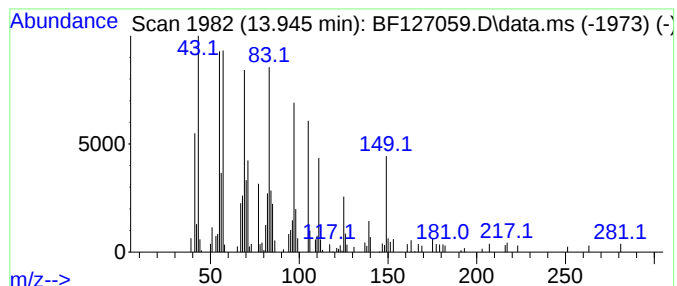
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Peak Number 4 n-Nonadecanol-1 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	10.73 ng	231913	Chrysene-d12	14.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Nonadecanol-1	284	C19H40O	001454-84-8	93
2			1-Heneicosanol	312	C21H44O	015594-90-8	93
3			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	91
4			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
5			1-Hexacosene	364	C26H52	018835-33-1	89



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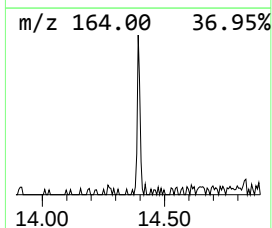
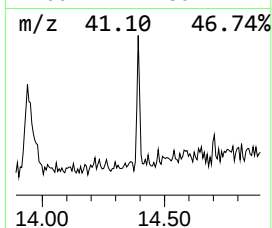
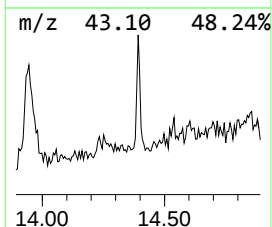
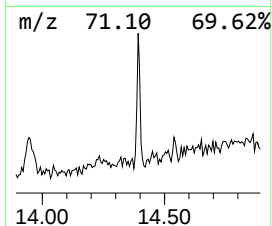
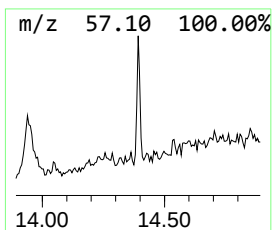
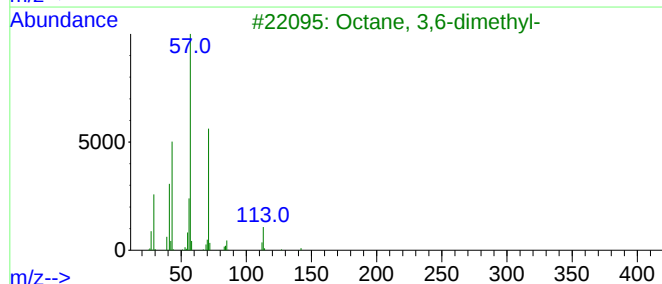
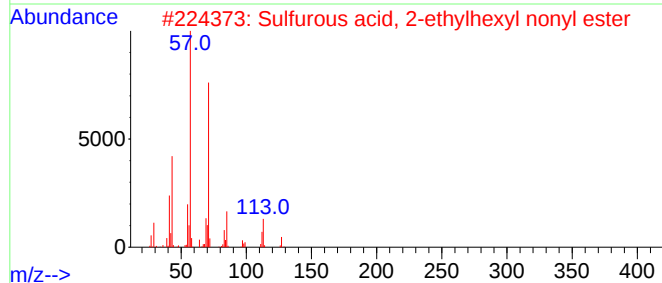
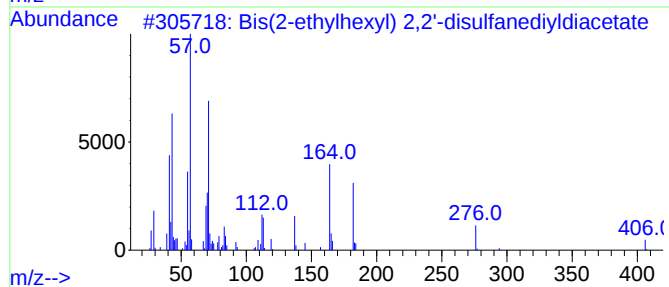
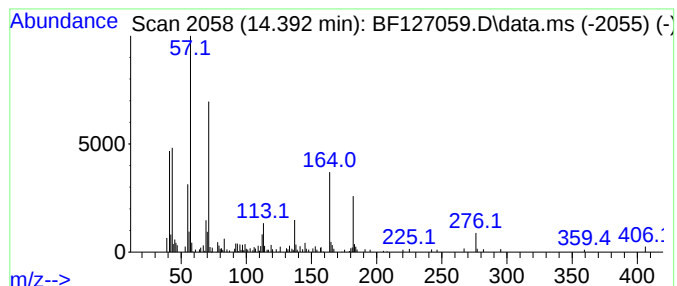
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Peak Number 5 Bis(2-ethylhexyl) 2,2'-disu... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.392	3.23 ng	69776	Chrysene-d12	14.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bis(2-ethylhexyl) 2,2'-disulfane...	406	C20H38O4S2	062268-47-7	83
2			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	43
3			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	38
4			Octane, 1-iodo-	240	C8H17I	000629-27-6	38
5			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
7-Tetradecene	9.757	2.2	ng	70762	3	9.945	640119	20.0
1,2-Benzenedica...	11.598	54.8	ng	1839220	4	11.439	671425	20.0
n-Hexadecanoic ...	11.951	3.7	ng	125332	4	11.439	671425	20.0
n-Nonadecanol-1	13.945	10.7	ng	231913	5	14.086	432079	20.0
Bis(2-ethylhexy...	14.392	3.2	ng	69776	5	14.086	432079	20.0