

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032521\
 Data File : BF123466.D
 Acq On : 25 Mar 2021 17:39
 Operator : JU/CG
 Sample : M1786-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1

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-BF032321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123466.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	14	22	28	rVB	1416889	1777103	28.35%	4.175%
2	2.322	35	40	46	rBV	87714	113605	1.81%	0.267%
3	5.134	515	518	523	rVB	90510	107865	1.72%	0.253%
4	5.522	578	584	587	rBV	5652928	5710616	91.11%	13.417%
5	6.522	748	754	757	rBV	5310772	5968207	95.22%	14.022%
6	6.898	814	818	821	rBV	1634092	1267996	20.23%	2.979%
7	7.463	908	914	917	rBV	3631222	3856852	61.54%	9.062%
8	8.180	1031	1036	1040	rBV	1814457	1648822	26.31%	3.874%
9	9.263	1215	1220	1223	rBV	7366860	6267516	100.00%	14.725%
10	9.651	1283	1286	1290	rBV	232028	182110	2.91%	0.428%
11	9.939	1331	1335	1339	rVB	2202621	1815195	28.96%	4.265%
12	10.239	1383	1386	1389	rBV	303930	239630	3.82%	0.563%
13	10.727	1465	1469	1473	rBV	3902378	3665180	58.48%	8.611%
14	11.427	1585	1588	1592	rBV	1906857	1599765	25.52%	3.759%
15	11.957	1673	1678	1681	rBV	370906	319239	5.09%	0.750%
16	12.745	1809	1812	1817	rBV	113571	120596	1.92%	0.283%
17	13.021	1855	1859	1862	rBV	5163723	4620202	73.72%	10.855%
18	13.562	1948	1951	1955	rBV	261895	232181	3.70%	0.546%
19	13.933	2011	2014	2025	rBV2	316784	605793	9.67%	1.423%
20	14.074	2034	2038	2042	rBV	1199279	1038702	16.57%	2.440%
21	15.527	2282	2285	2289	rBV	273130	342827	5.47%	0.805%
22	15.574	2289	2293	2297	rVB	895094	1062873	16.96%	2.497%

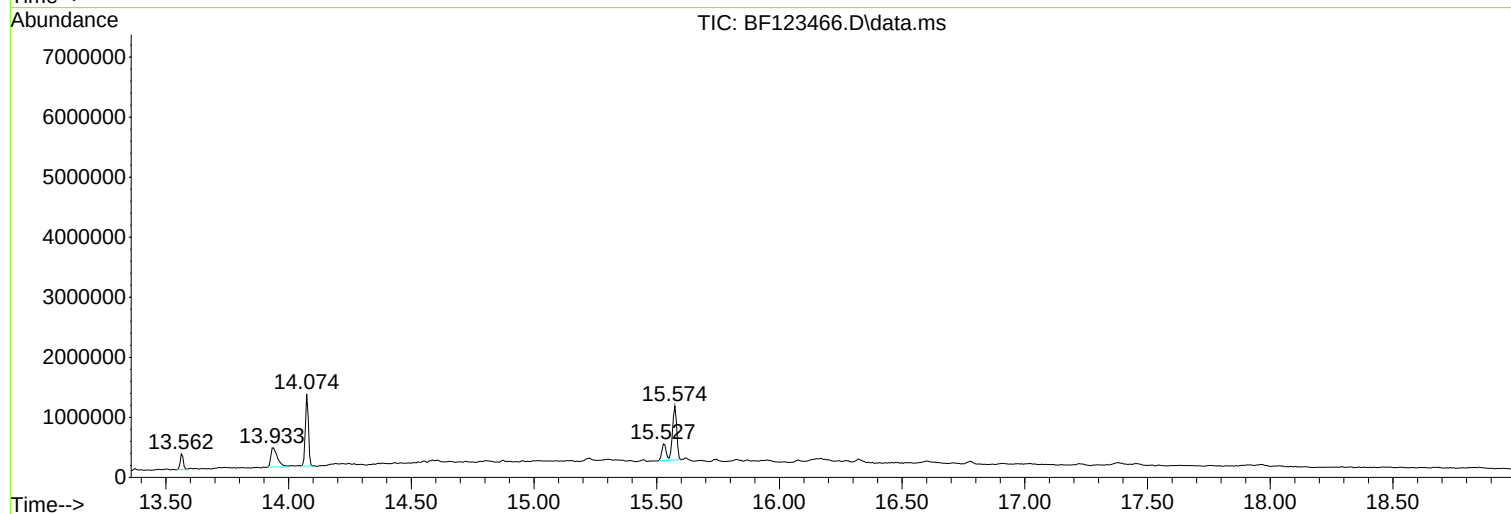
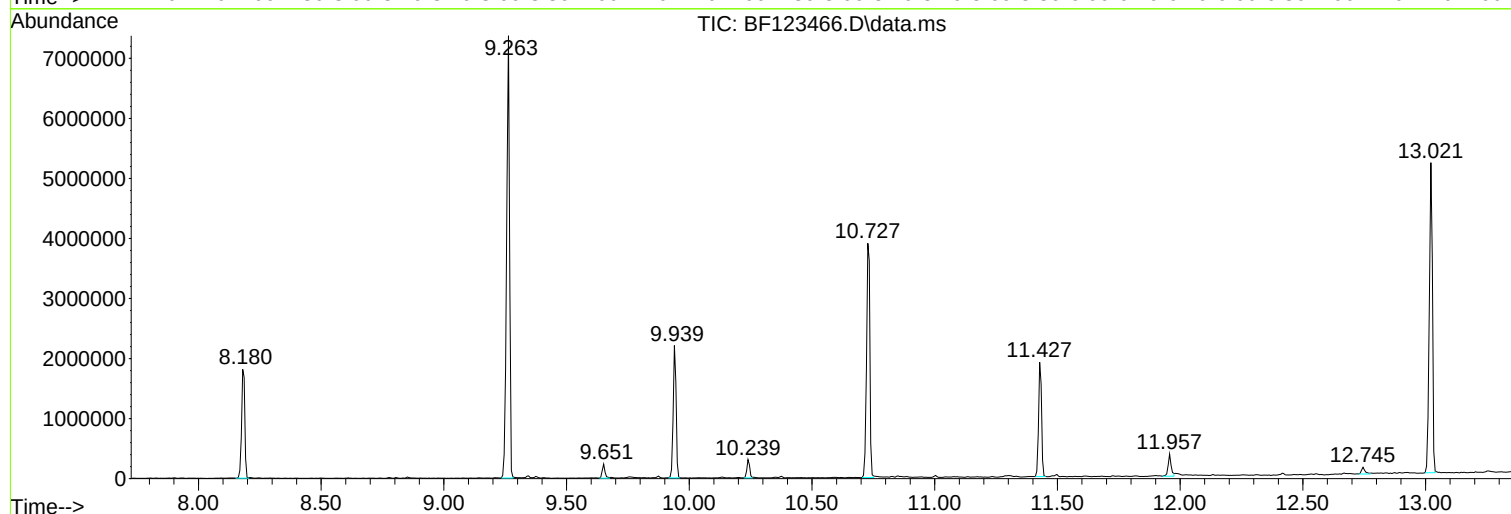
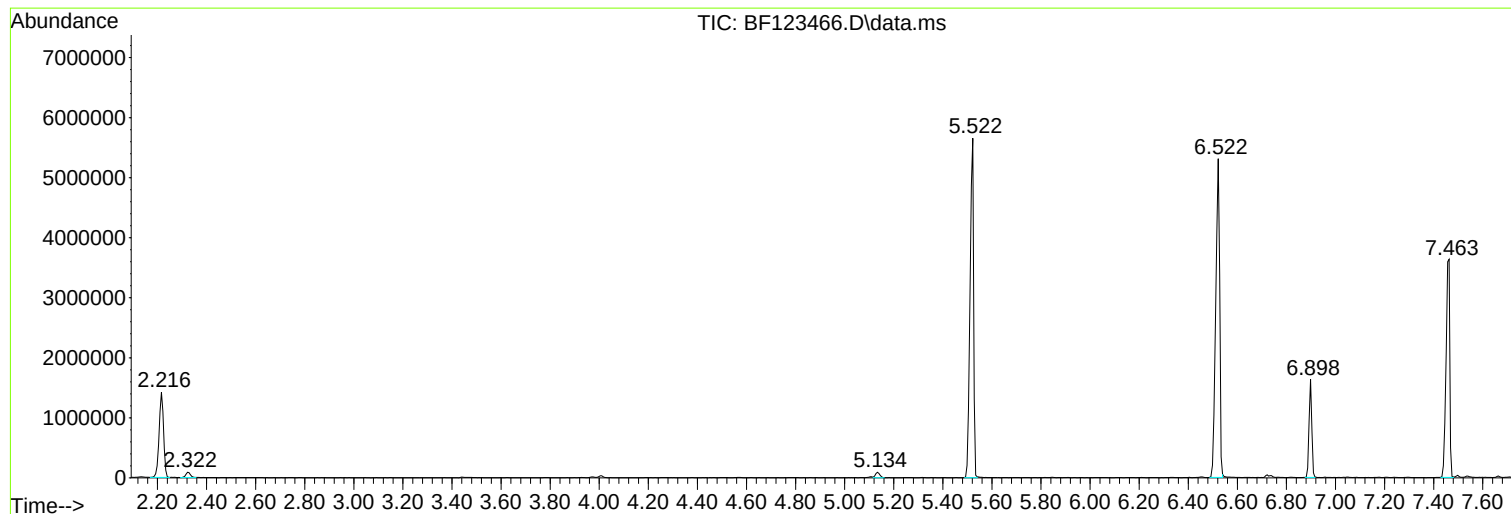
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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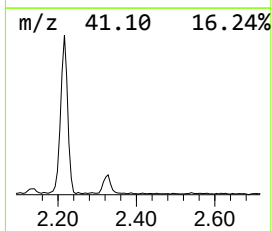
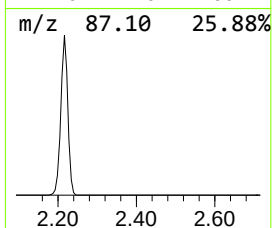
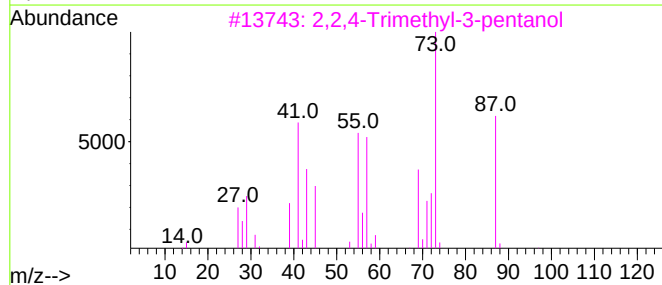
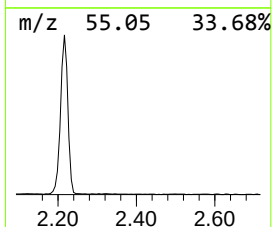
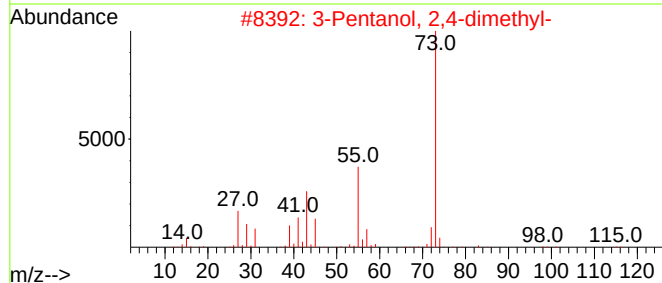
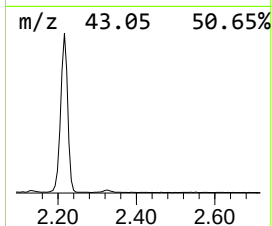
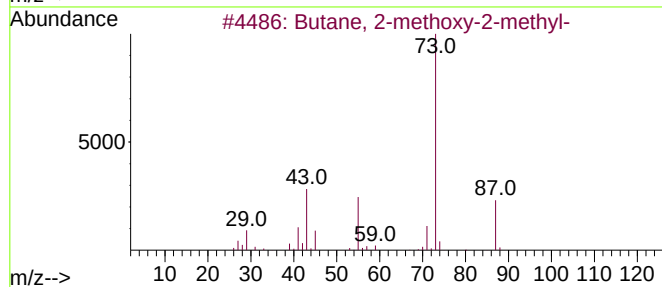
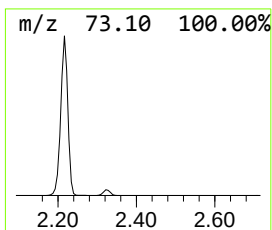
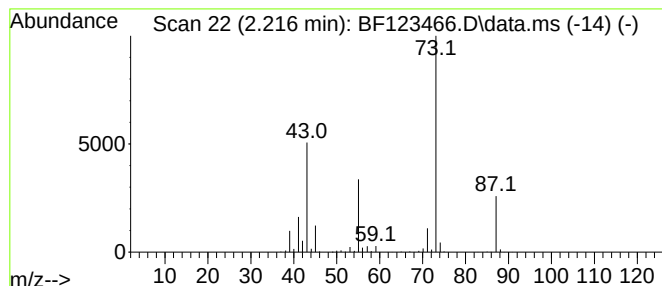
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	28.03 ng	1777100	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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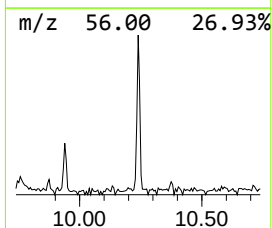
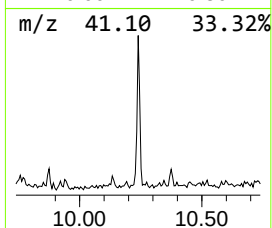
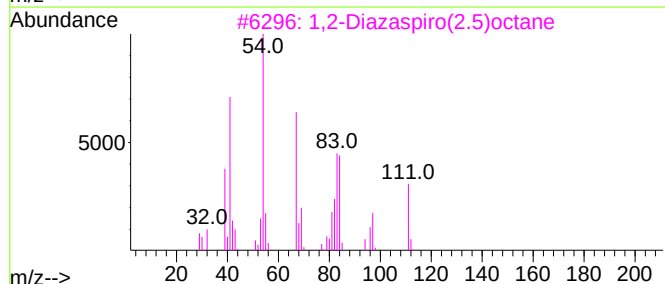
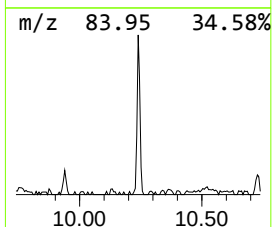
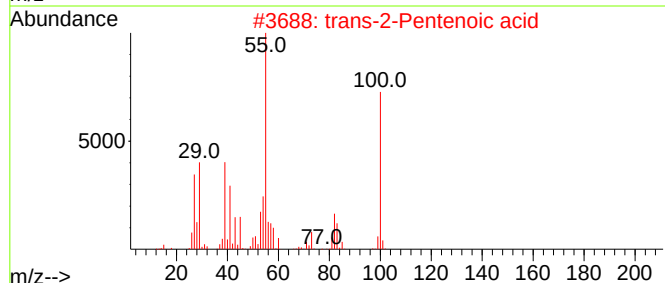
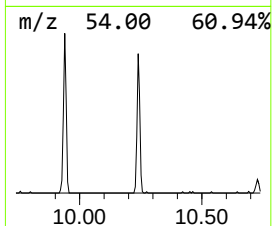
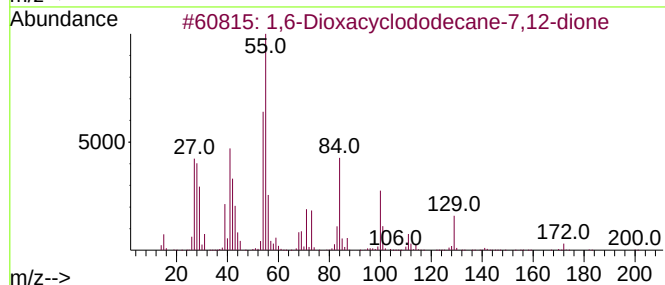
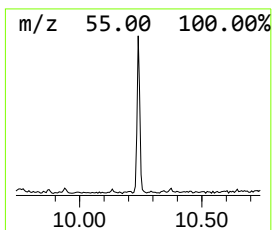
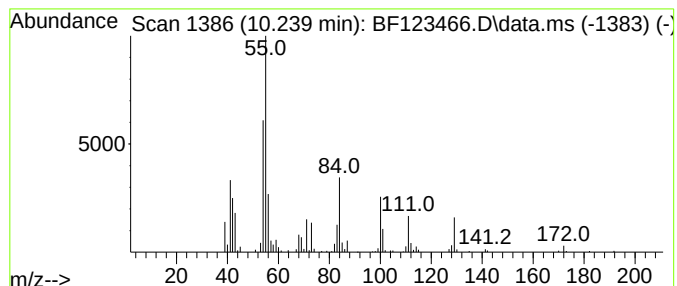
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1,6-Dioxacyclododecane-7,12... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.239	2.64 ng	239630	Acenaphthene-d10	9.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,6-Dioxacyclododecane-7,12-dione	200	C10H16O4	000777-95-7	91
2			trans-2-Pentenoic acid	100	C5H8O2	013991-37-2	38
3			1,2-Diazaspiro(2.5)octane	112	C6H12N2	000185-79-5	27
4			4-Pentenoic acid	100	C5H8O2	000591-80-0	25
5			Ethanamine, N-cyclopentylidene-	111	C7H13N	054966-05-1	25



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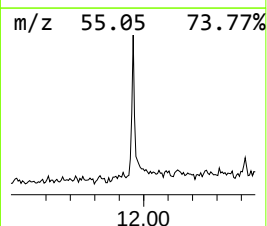
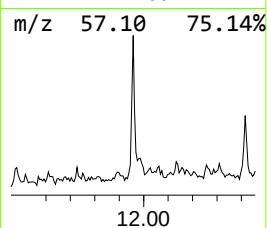
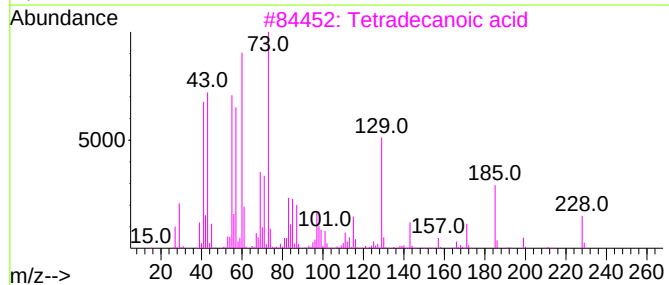
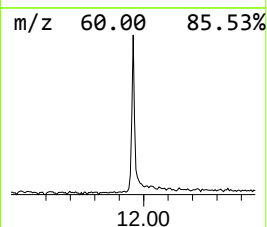
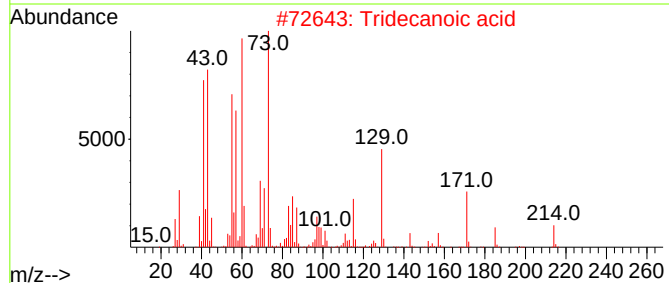
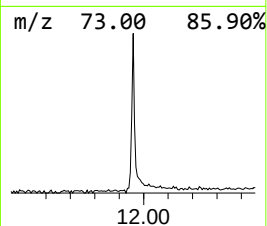
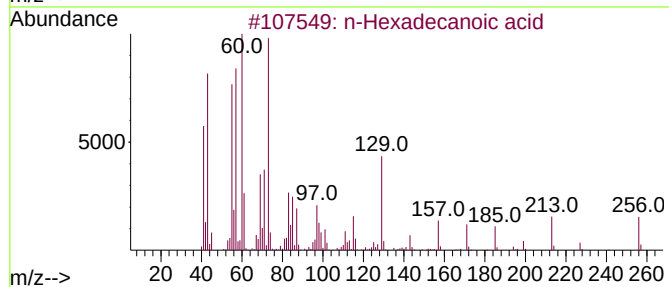
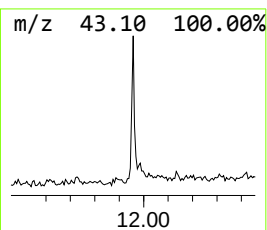
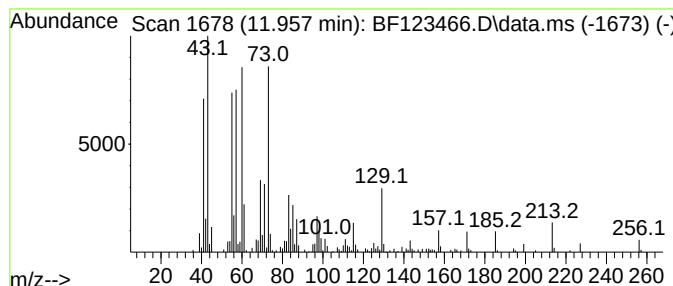
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	3.99 ng	319239	Phenanthrene-d10	11.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	78



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Instrument :
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ClientSampled :
SP-1

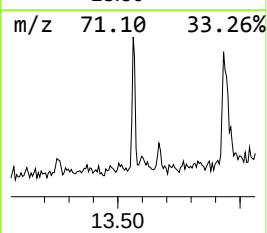
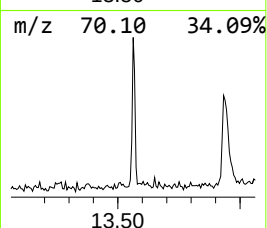
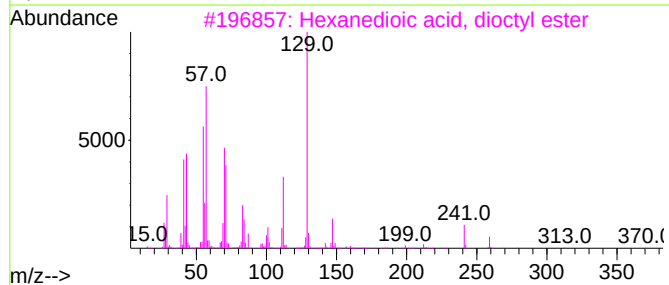
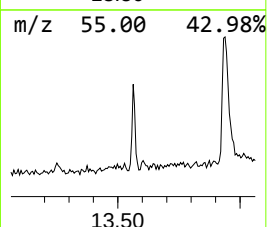
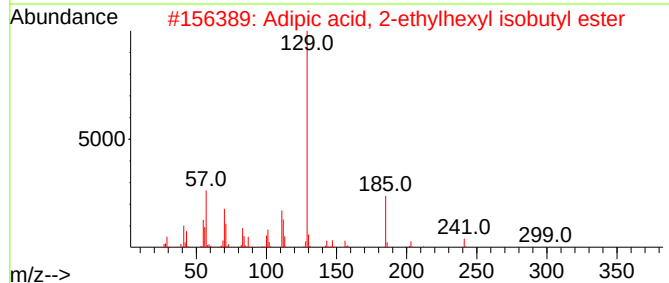
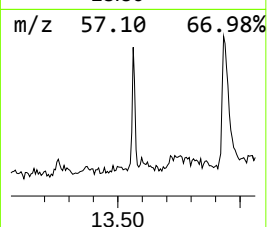
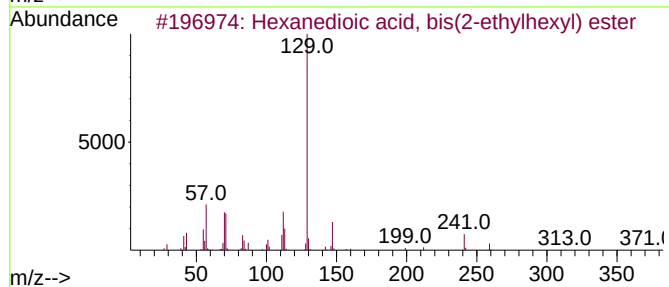
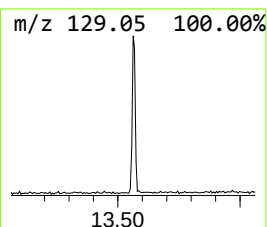
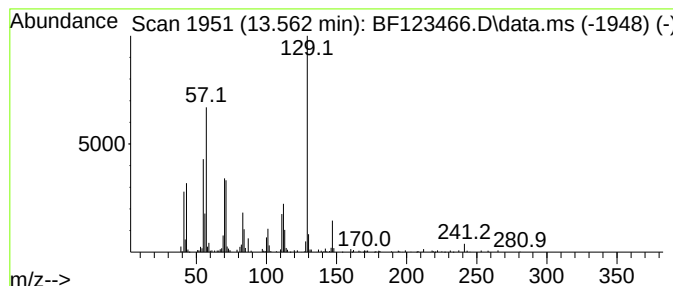
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Hexanedioic acid, bis(2-eth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.563	4.47 ng	232181	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	90
2			Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1000324-48-0	72
3			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	70
4			Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	64
5			Diisooctyl adipate	370	C22H42O4	001330-86-5	58



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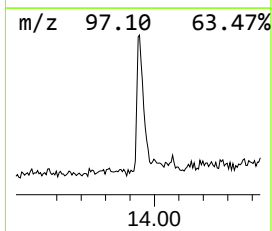
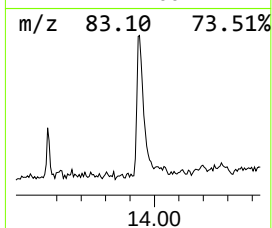
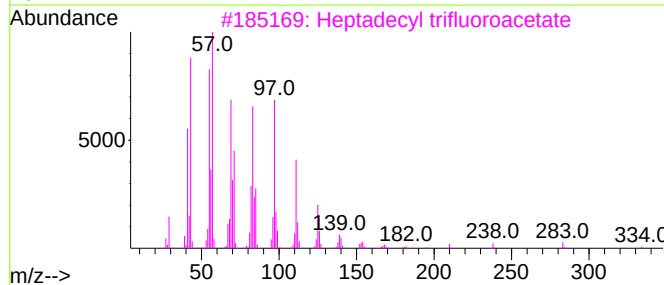
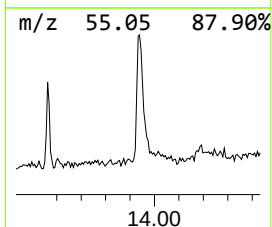
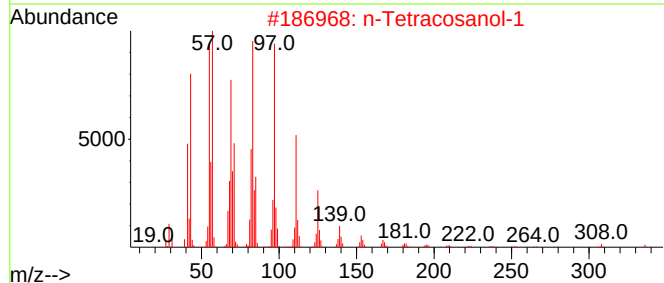
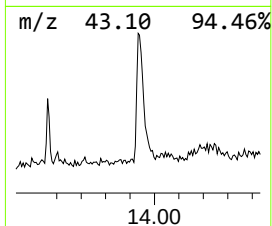
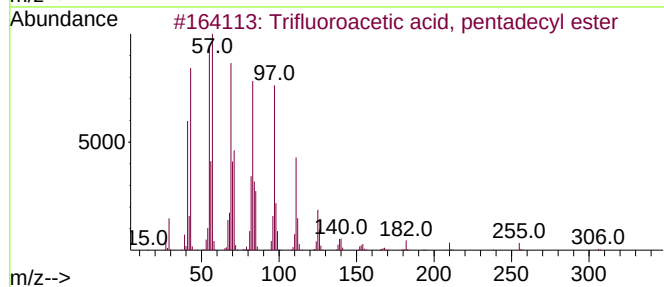
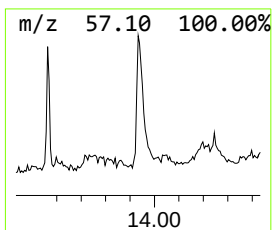
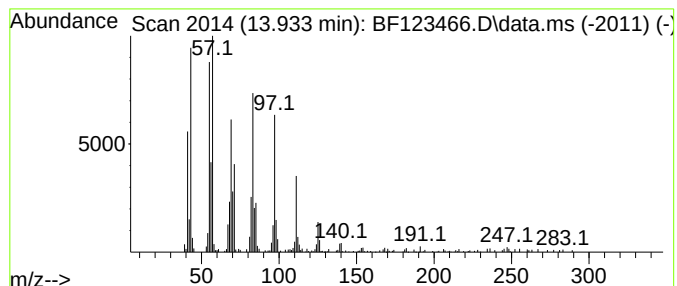
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Trifluoroacetic acid, penta... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	11.66 ng	605793	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.216	28.0	ng	1777100	1	6.898	1268000	20.0
1,6-Dioxacyclod...	10.239	2.6	ng	239630	3	9.939	1815200	20.0
n-Hexadecanoic ...	11.957	4.0	ng	319239	4	11.427	1599770	20.0
Hexanedioic aci...	13.563	4.5	ng	232181	5	14.074	1038700	20.0
Trifluoroacetic...	13.933	11.7	ng	605793	5	14.074	1038700	20.0