

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
 Data File : BF123488.D
 Acq On : 26 Mar 2021 16:08
 Operator : JU/CG
 Sample : M1770-13
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-103D

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: BF123488.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.246	20	27	33	rVB	3511231	4460782	53.16%	8.507%
2	2.352	41	45	54	rVB	105850	130683	1.56%	0.249%
3	5.122	508	516	525	rVB	75410	103466	1.23%	0.197%
4	5.516	578	583	586	rBV	3919455	3688357	43.95%	7.034%
5	6.516	748	753	763	rBV	3314165	3334780	39.74%	6.360%
6	6.898	814	818	821	rBV	1849190	1495951	17.83%	2.853%
7	7.463	907	914	917	rBV	4696813	4939153	58.86%	9.420%
8	8.181	1031	1036	1040	rBV	1949335	1949165	23.23%	3.717%
9	8.575	1097	1103	1111	rBV	490707	602564	7.18%	1.149%
10	9.263	1214	1220	1223	rBV	8066974	8391559	100.00%	16.004%
11	9.651	1283	1286	1290	rBV	132496	101919	1.21%	0.194%
12	9.775	1300	1307	1318	rBV4	58742	175485	2.09%	0.335%
13	9.939	1327	1335	1339	rBV	2280020	2225616	26.52%	4.245%
14	10.145	1366	1370	1377	rVB	365700	324140	3.86%	0.618%
15	10.733	1464	1470	1473	rBV	5614681	5658402	67.43%	10.792%
16	11.433	1583	1589	1592	rBV	2498917	2151479	25.64%	4.103%
17	11.957	1673	1678	1686	rBV2	454613	481320	5.74%	0.918%
18	12.416	1753	1756	1759	rVB	114159	96222	1.15%	0.184%
19	12.668	1796	1799	1809	rBV	109767	135042	1.61%	0.258%
20	12.745	1809	1812	1821	rVV	92438	95608	1.14%	0.182%
21	13.027	1853	1860	1863	rBV	7680518	8292864	98.82%	15.816%
22	13.874	1998	2004	2007	rBV	99723	148894	1.77%	0.284%
23	13.915	2007	2011	2013	rBV	127986	152460	1.82%	0.291%
24	13.945	2013	2016	2024	rVB2	429429	600362	7.15%	1.145%
25	14.080	2035	2039	2042	rVB	1740289	1493129	17.79%	2.848%
26	15.580	2288	2294	2298	rBV	935939	1204133	14.35%	2.296%

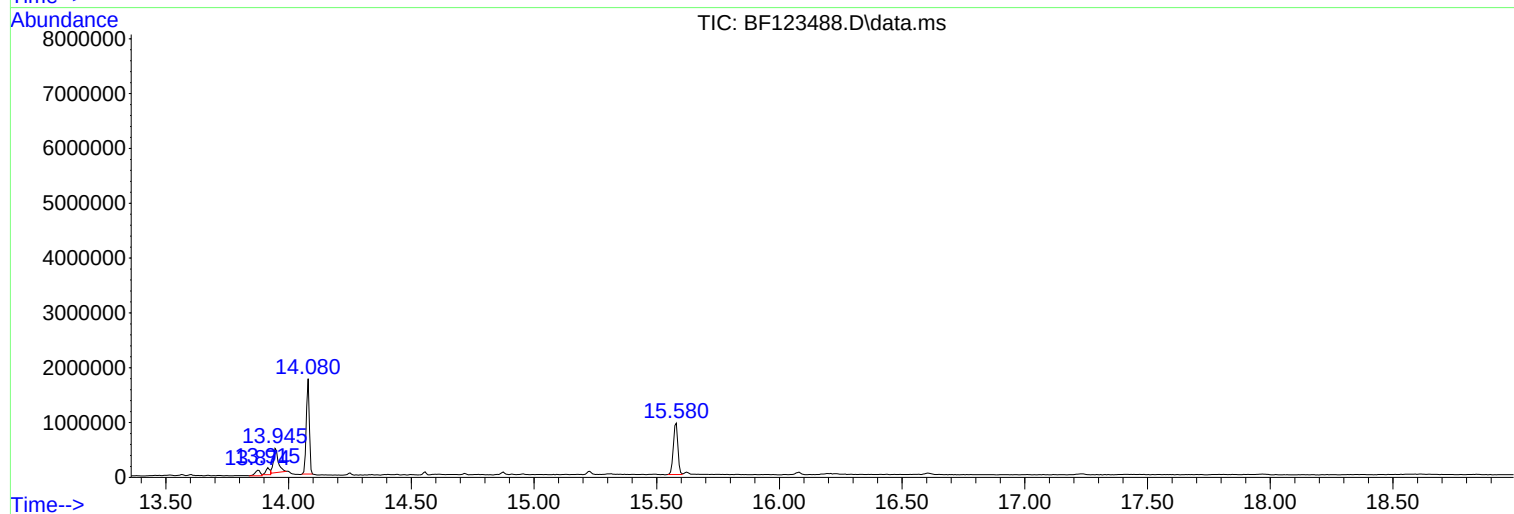
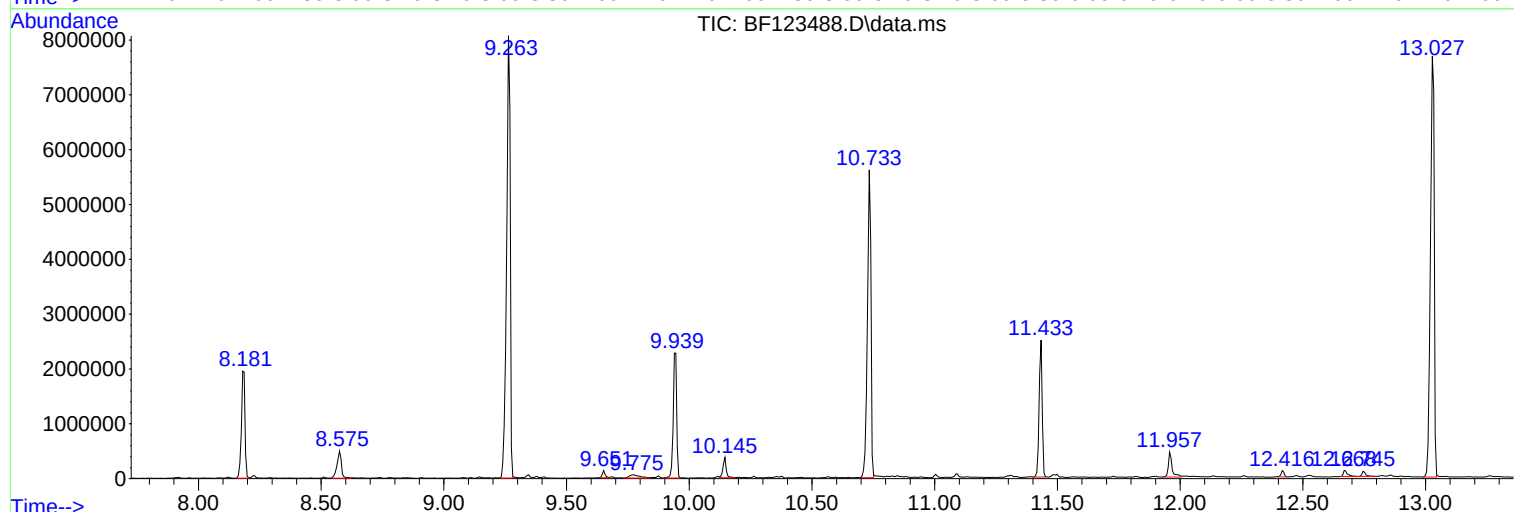
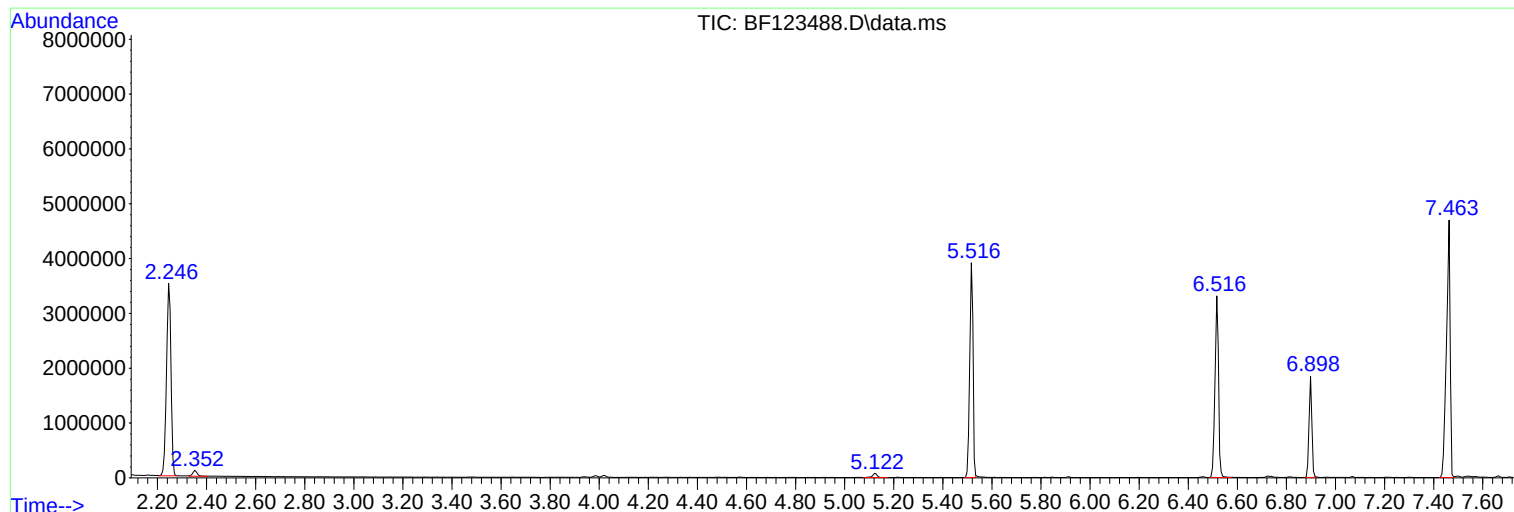
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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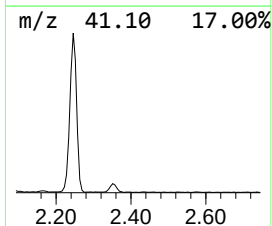
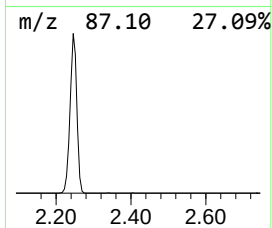
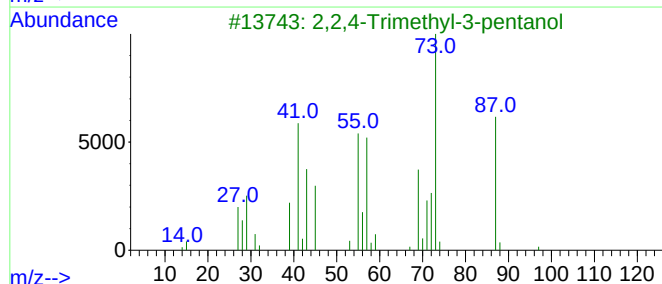
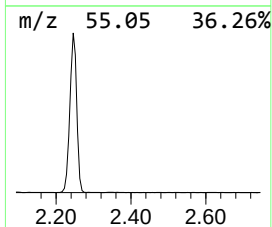
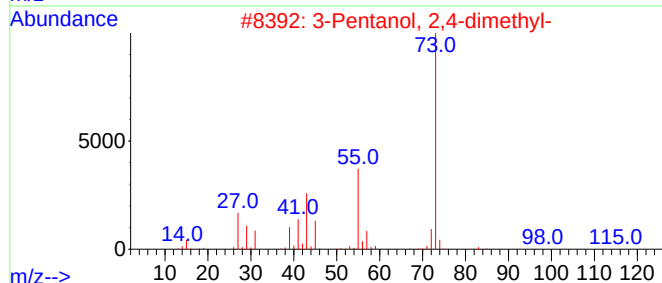
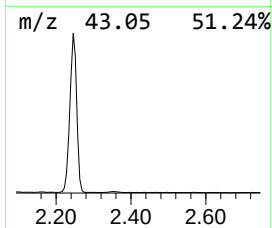
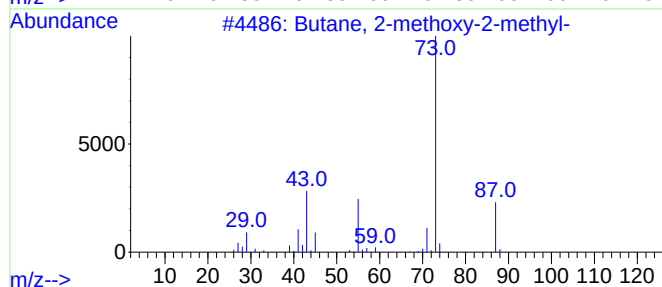
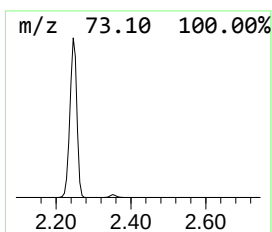
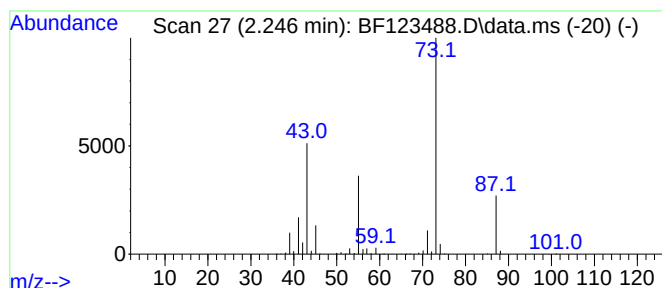
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.246	59.64 ng	4460780	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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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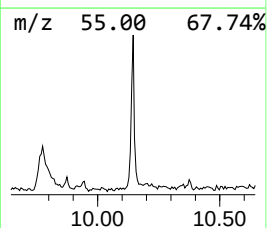
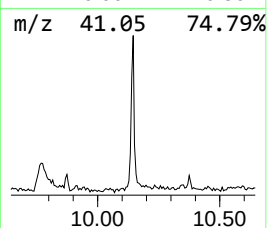
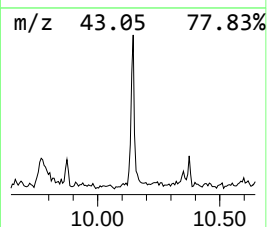
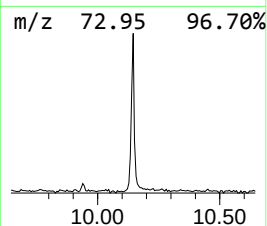
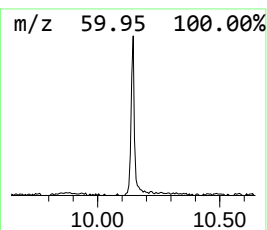
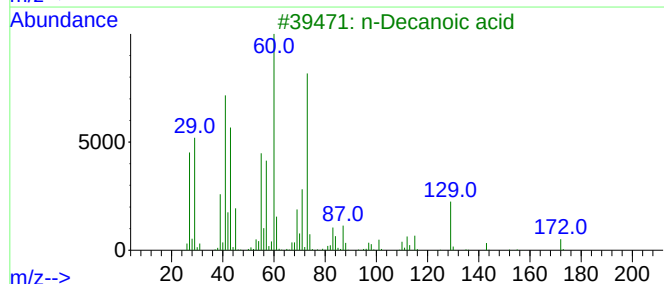
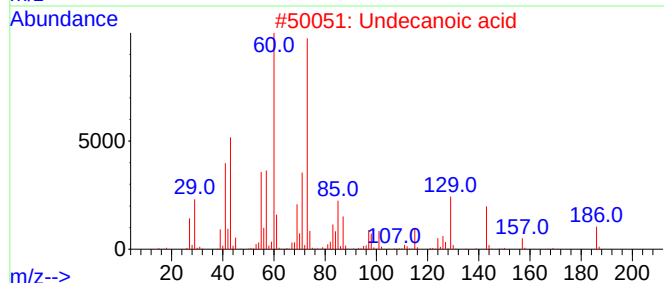
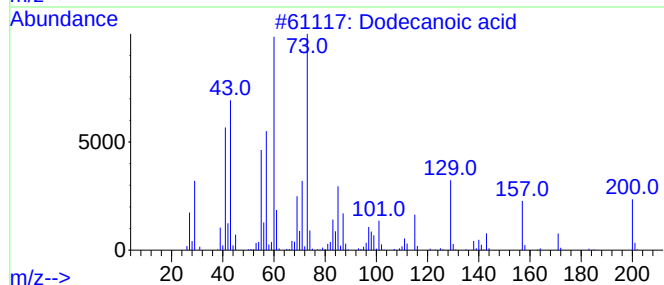
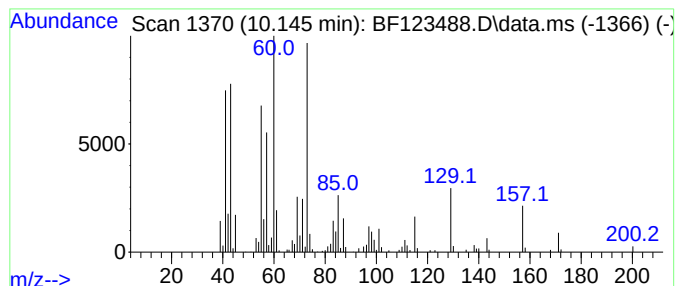
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Dodecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.145	2.91 ng	324140	Acenaphthene-d10	9.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	91
2			Undecanoic acid	186	C11H22O2	000112-37-8	78
3			n-Decanoic acid	172	C10H20O2	000334-48-5	76
4			Nonanoic acid	158	C9H18O2	000112-05-0	52
5			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	40



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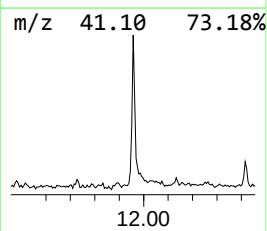
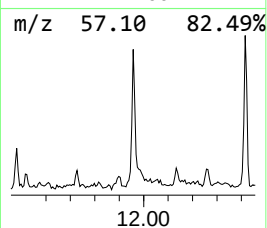
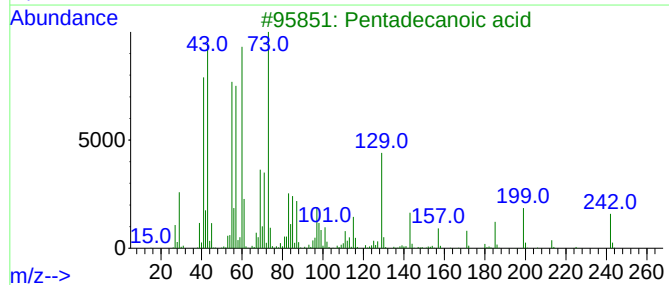
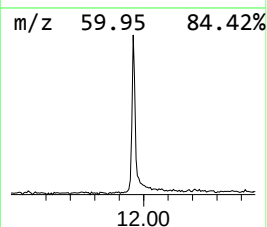
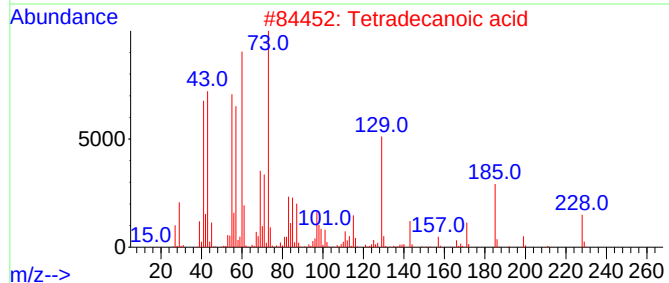
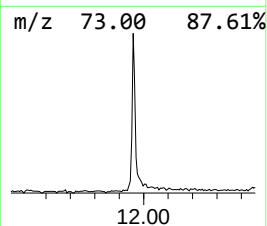
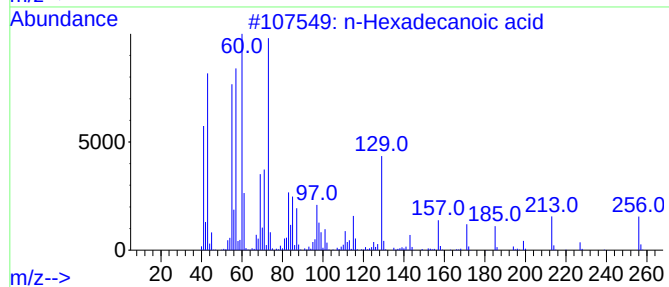
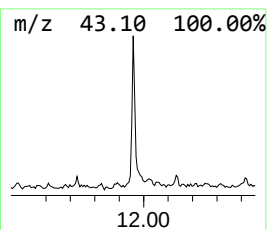
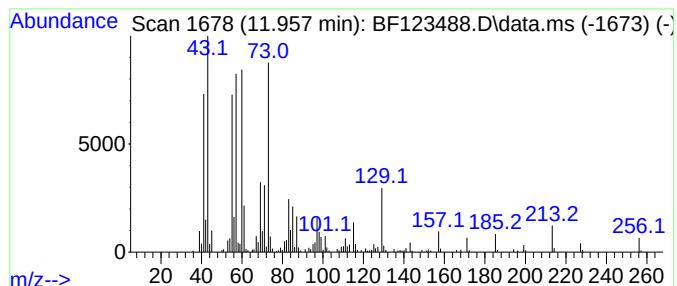
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	4.47 ng	481320	Phenanthrene-d10	11.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tridecanoic acid	214	C13H26O2	000638-53-9	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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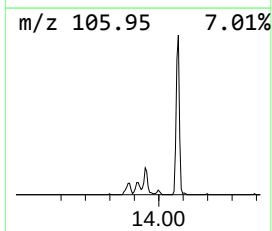
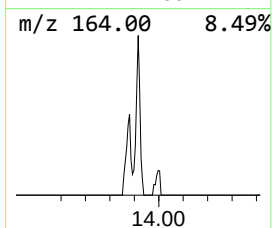
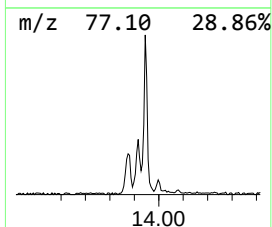
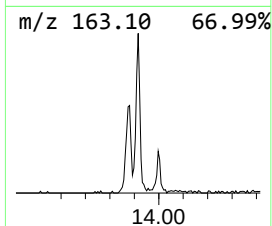
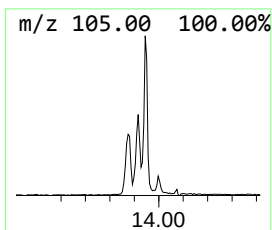
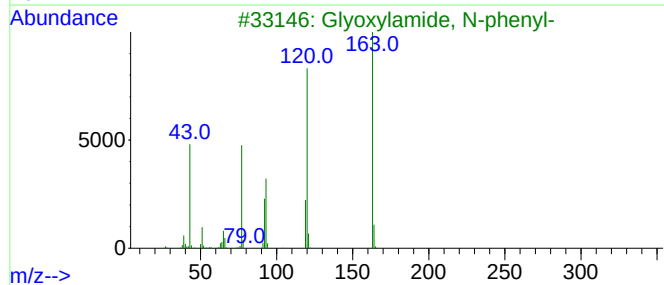
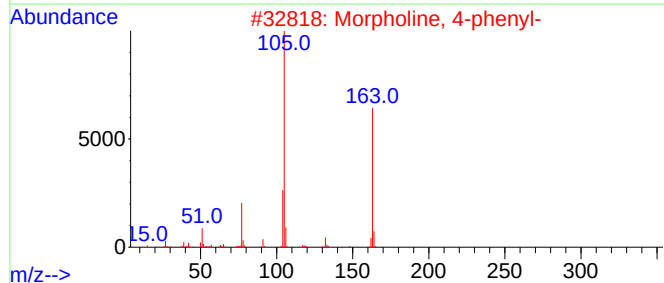
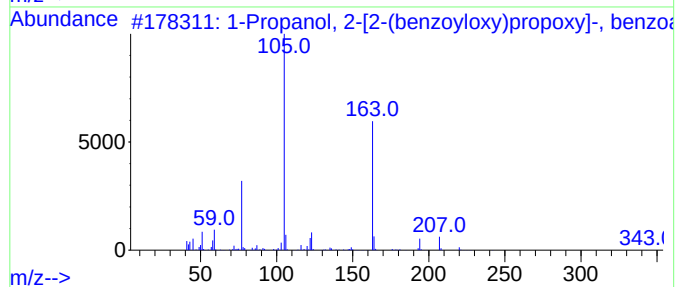
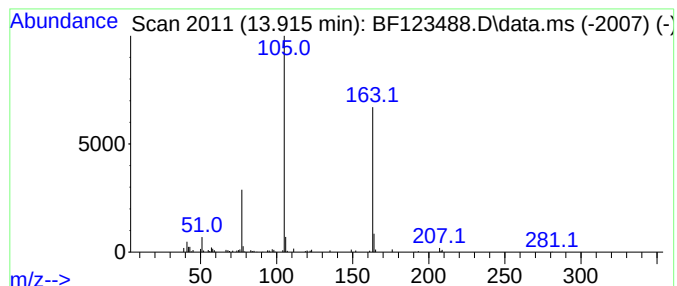
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Propanol, 2-[2-(benzoylox... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.916	2.04 ng	152460	Chrysene-d12	14.080	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	72
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	59
3	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	47
4	.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	38
5	4-Chlorophenyl benzoate	232	C13H9ClO2	002005-08-5	27



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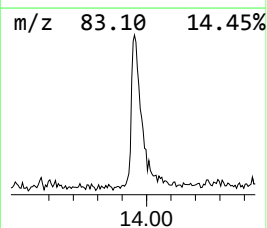
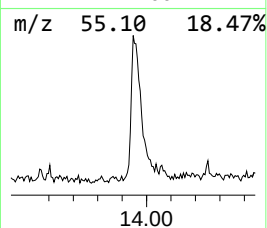
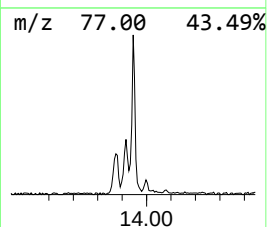
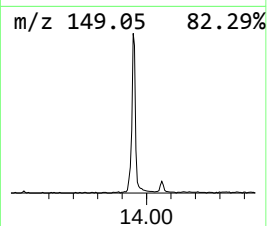
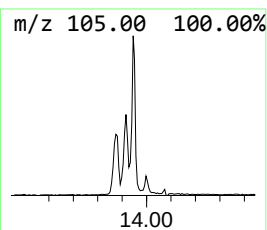
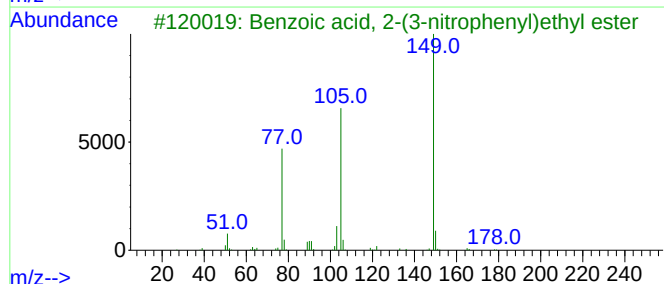
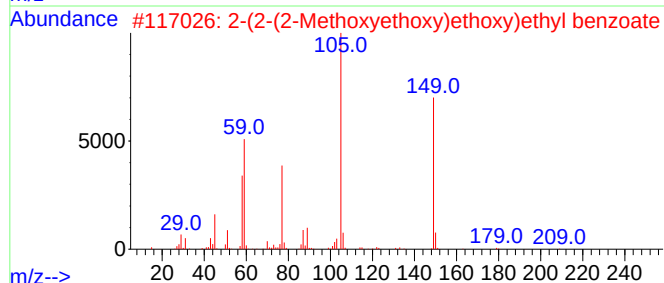
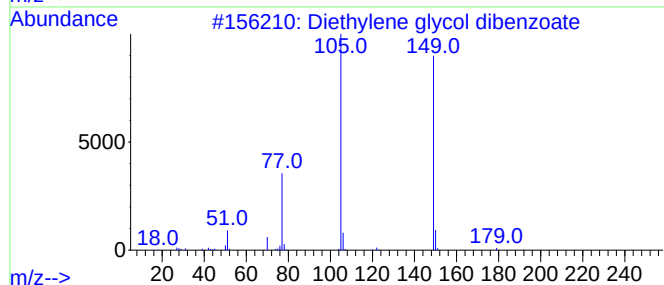
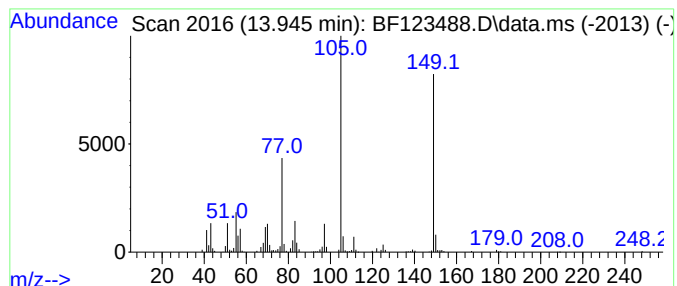
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	8.04 ng	600362	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
2			2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	64
3			Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	59
4			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	46
5			Phthalic acid, isobutyl pentadec...	432	C27H44O4	1000309-07-3	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.246	59.6	ng	4460780	1	6.898	1495950	20.0
Dodecanoic acid	10.145	2.9	ng	324140	3	9.945	2225620	20.0
n-Hexadecanoic ...	11.957	4.5	ng	481320	4	11.433	2151480	20.0
1-Propanol, 2-[...	13.916	2.0	ng	152460	5	14.080	1493130	20.0
Diethylene glyc...	13.945	8.0	ng	600362	5	14.080	1493130	20.0