

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090421\
 Data File : BF125372.D
 Acq On : 4 Sep 2021 16:44
 Operator : JU/CG
 Sample : M3648-08
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20211057-SI-COMP-2-MODIFIED-EL

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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125372.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	10	18	31	rVB	3074275	4143780	94.70%	14.292%
2	5.516	579	583	587	rBV	2357801	2243495	51.27%	7.738%
3	6.522	750	754	767	rBV	1761444	1558305	35.61%	5.375%
4	6.898	814	818	821	rBV	1009040	853590	19.51%	2.944%
5	7.463	906	914	917	rBV	2713814	2700748	61.72%	9.315%
6	8.080	1016	1019	1032	rBV	92476	175099	4.00%	0.604%
7	8.180	1032	1036	1043	rVV	1261499	1057039	24.16%	3.646%
8	9.257	1214	1219	1222	rBV	4860268	4375698	100.00%	15.092%
9	9.933	1326	1334	1338	rBV	1305266	1155022	26.40%	3.984%
10	10.727	1464	1469	1472	rBV	2757103	2640456	60.34%	9.107%
11	11.421	1583	1587	1595	rBV	1190031	1020210	23.32%	3.519%
12	11.580	1611	1614	1618	rBV	1369092	1031087	23.56%	3.556%
13	11.804	1649	1652	1655	rVB2	111379	87482	2.00%	0.302%
14	11.939	1672	1675	1680	rBV2	169814	172815	3.95%	0.596%
15	12.727	1805	1809	1817	rBV	59796	72430	1.66%	0.250%
16	13.010	1852	1857	1860	rBV	3968351	3611963	82.55%	12.458%
17	13.927	2010	2013	2026	rBV	71174	105480	2.41%	0.364%
18	14.062	2032	2036	2042	rVB	916424	796524	18.20%	2.747%
19	15.556	2285	2290	2301	rVB	673928	941014	21.51%	3.246%
20	16.015	2364	2368	2376	rVB2	40507	57174	1.31%	0.197%
21	16.533	2450	2456	2463	rBV3	40147	79670	1.82%	0.275%
22	17.139	2555	2559	2567	rVB4	29972	61550	1.41%	0.212%
23	17.868	2677	2683	2690	rVB3	23708	53205	1.22%	0.184%

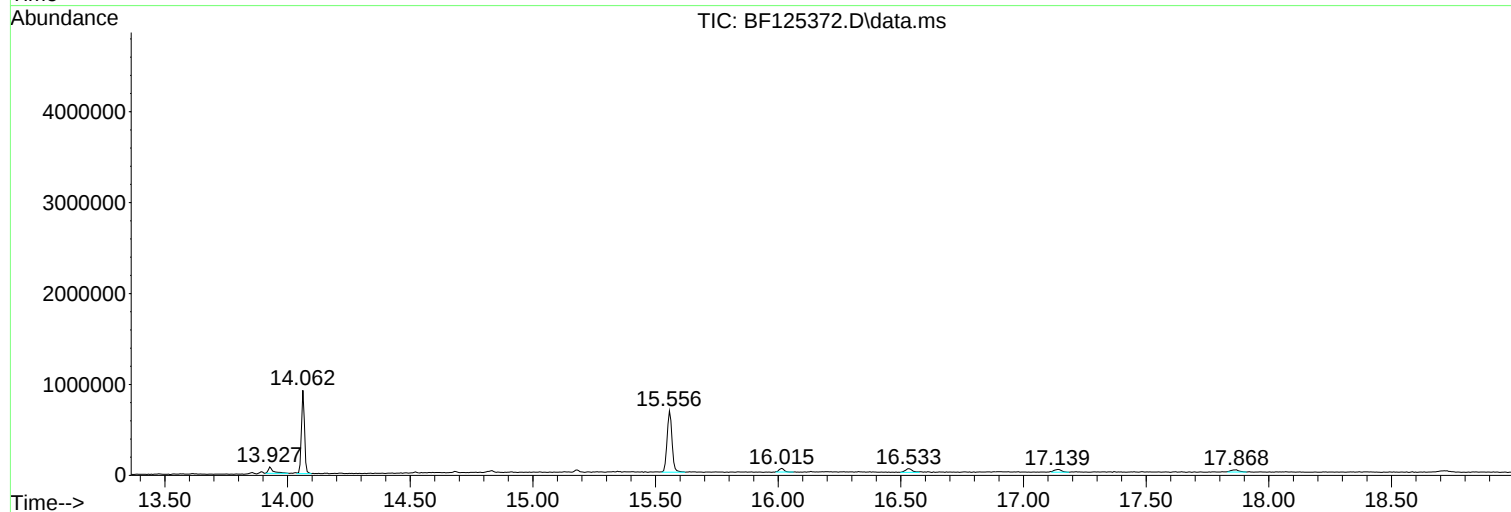
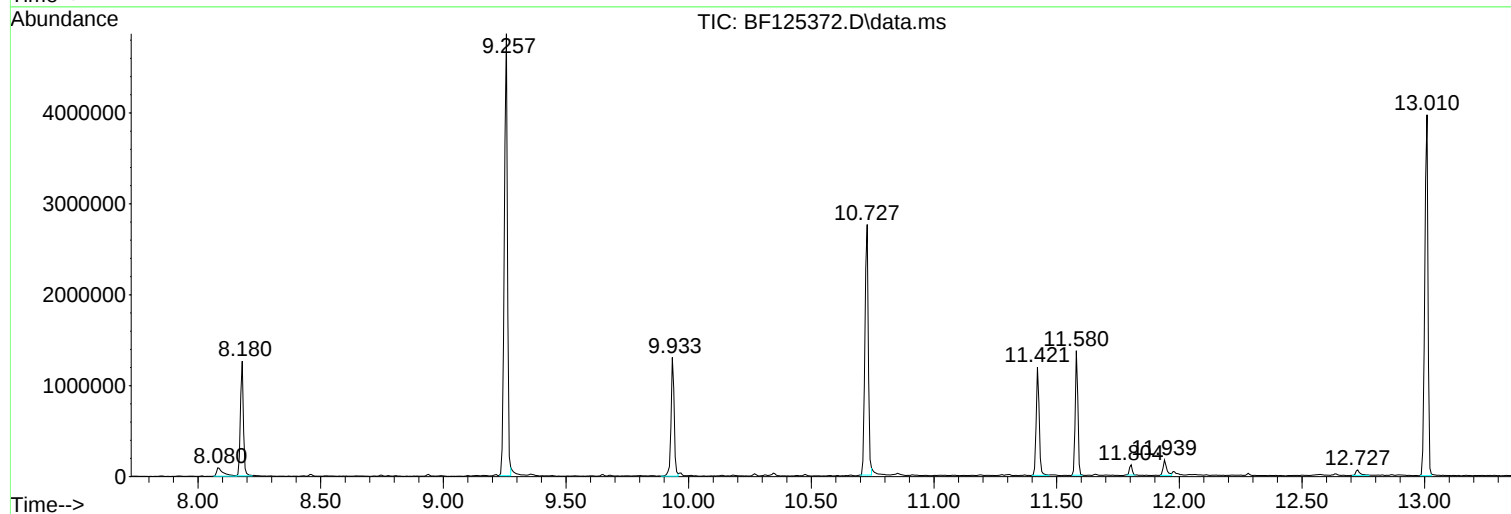
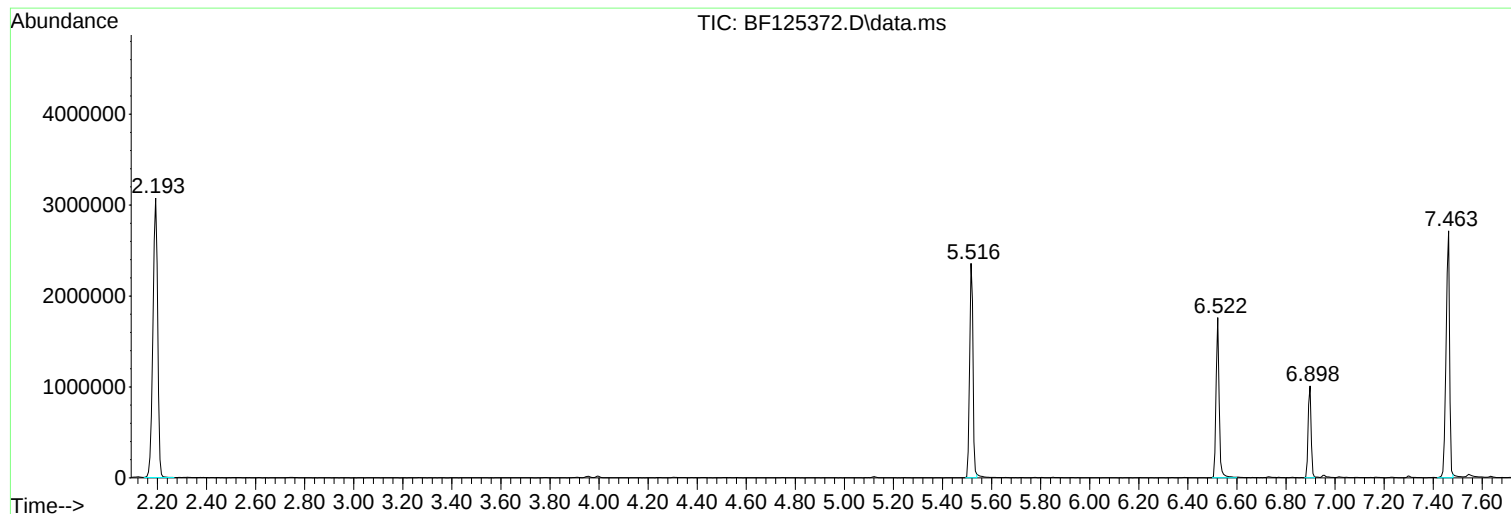
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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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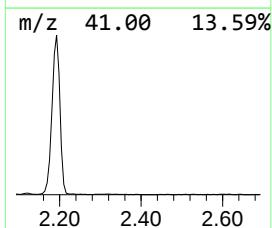
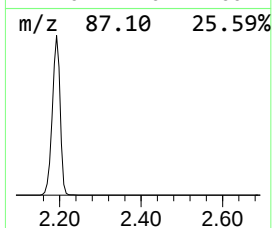
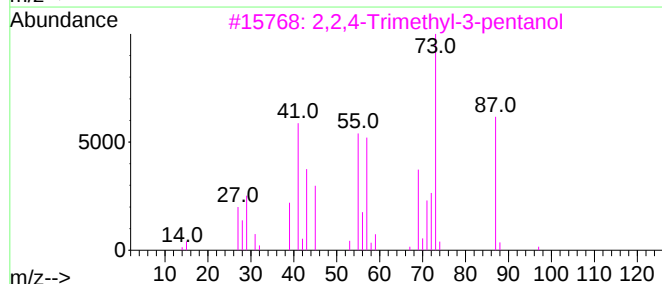
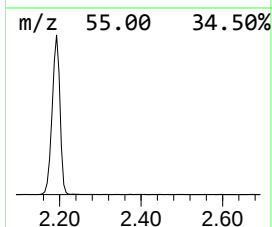
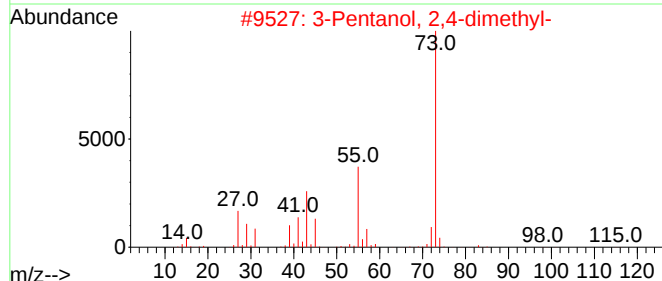
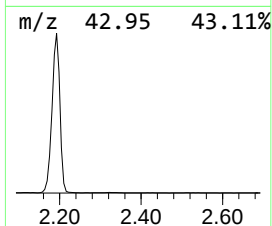
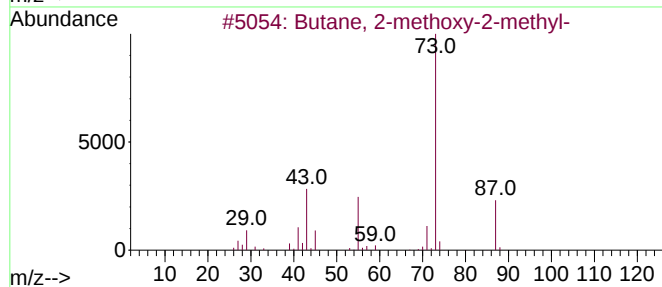
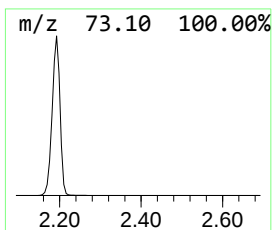
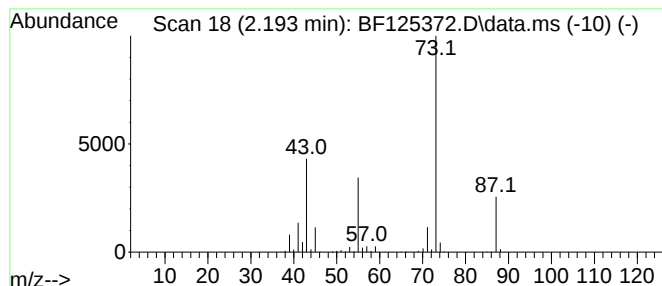
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	97.09 ng	4143780	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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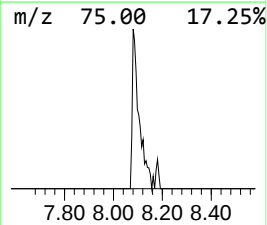
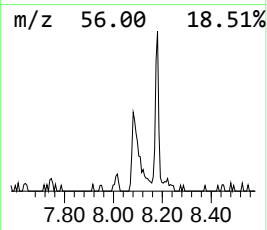
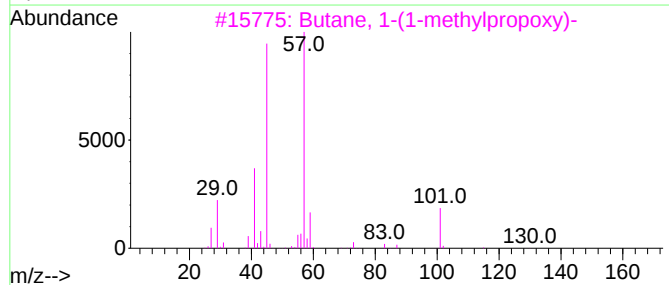
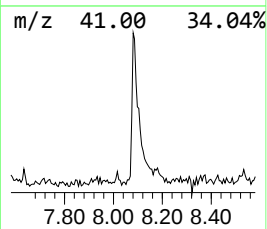
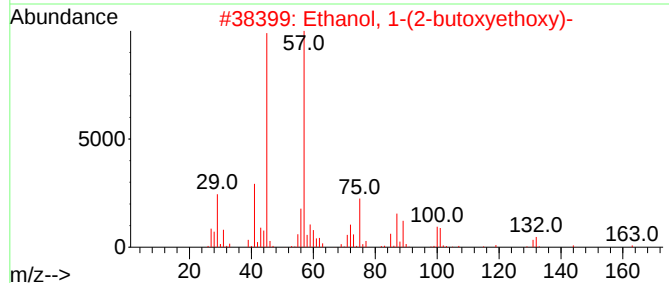
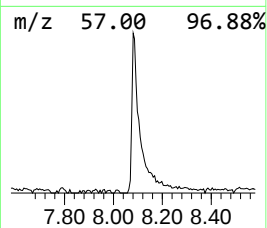
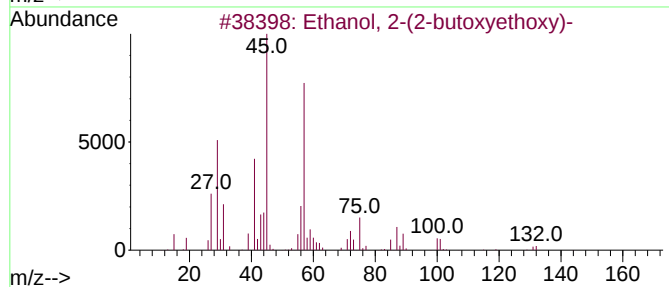
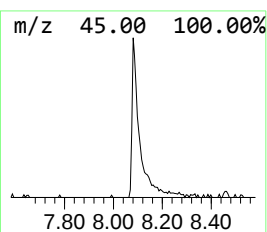
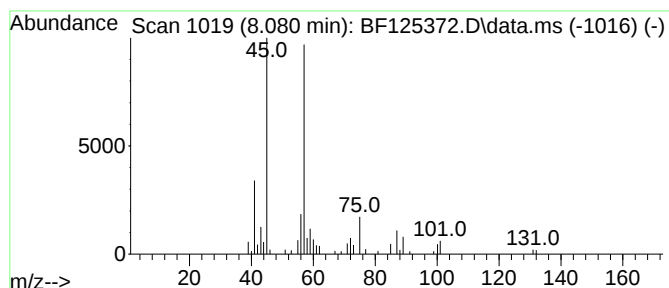
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.080	3.31 ng	175099	Naphthalene-d8	8.180

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	59
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53



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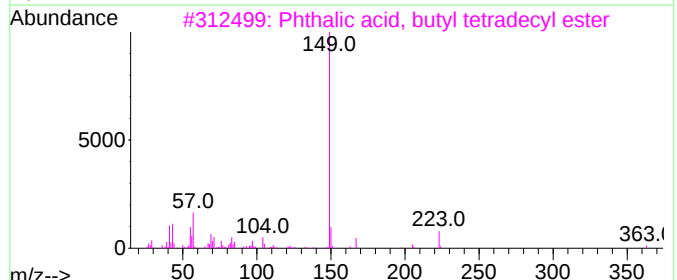
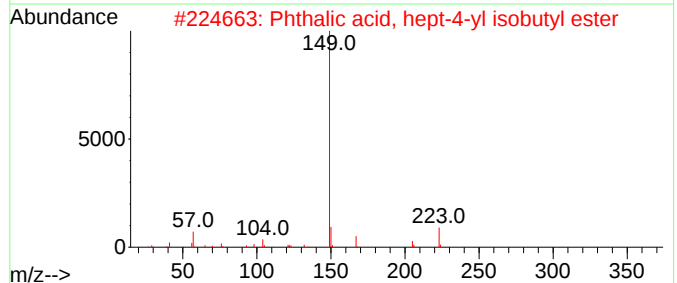
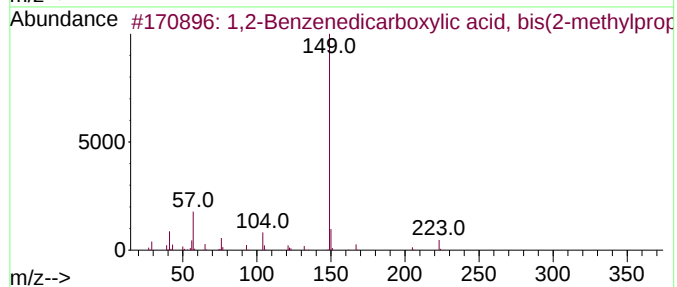
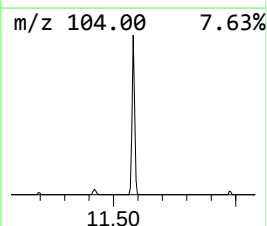
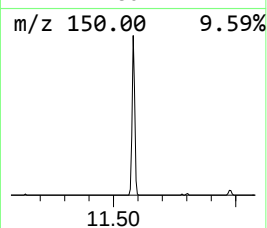
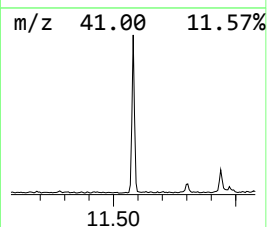
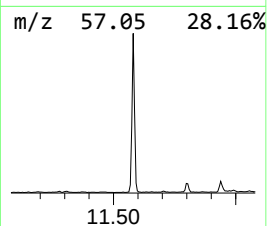
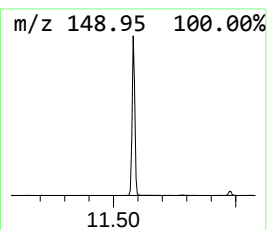
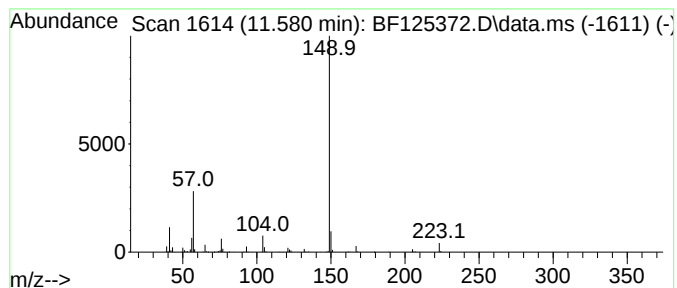
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Peak Number 3 1,2-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.580	20.21 ng	1031090	Phenanthrene-d10	11.421	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	90
2	Phthalic acid, hept-4-yl isobuty...	320	C19H28O4	1000356-78-3	83
3	Phthalic acid, butyl tetradecyl ...	418	C26H42O4	1000308-91-3	83
4	Phthalic acid, 8-bromooctyl isobu...	412	C20H29BrO4	1000382-55-3	83
5	1,2-Benzenedicarboxylic acid, bi...	250	C14H18O4	000605-45-8	78



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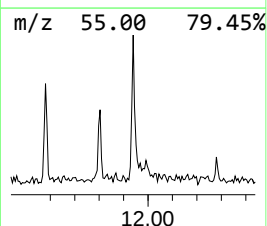
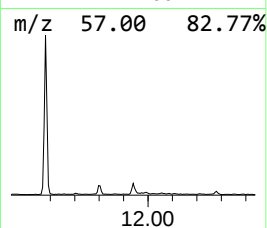
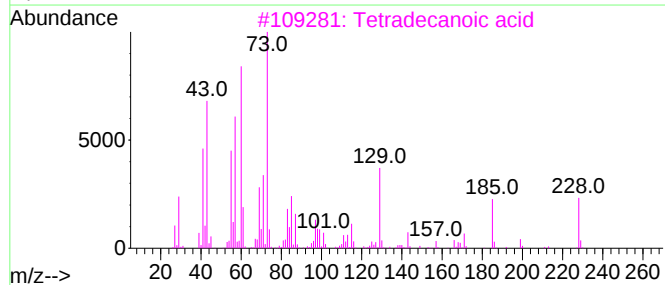
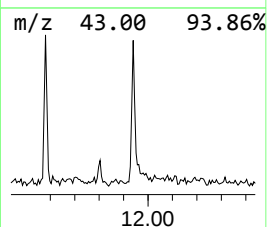
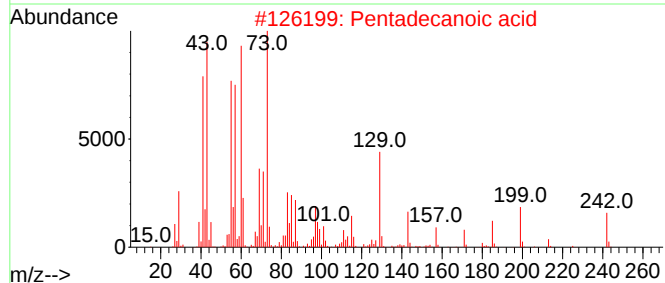
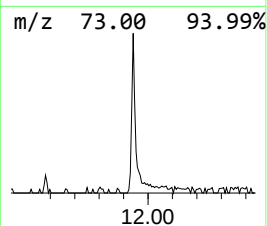
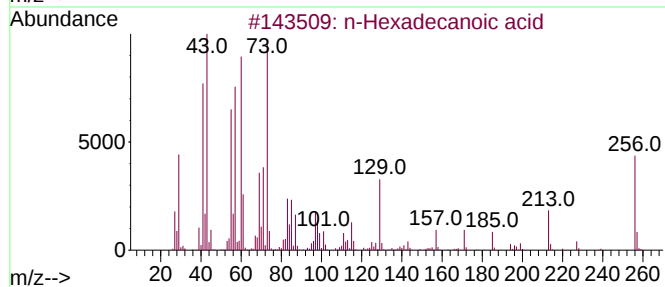
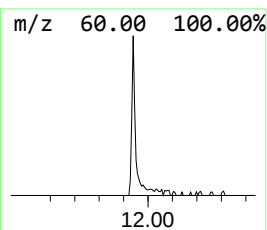
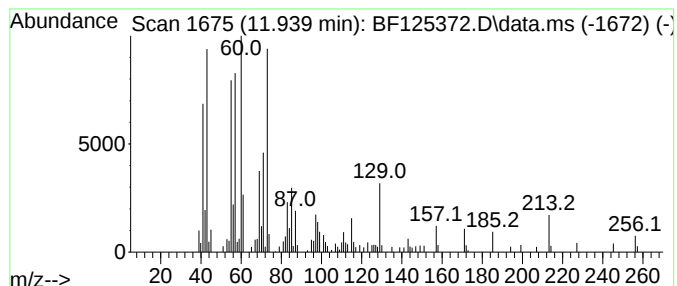
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	3.39 ng	172815	Phenanthrene-d10	11.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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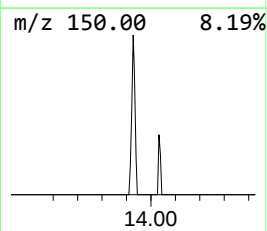
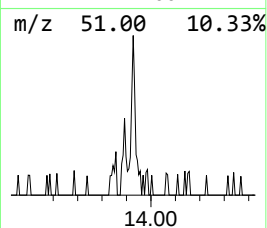
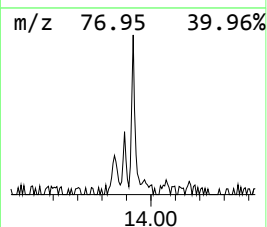
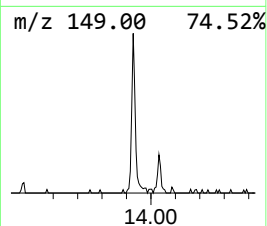
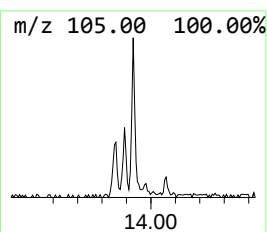
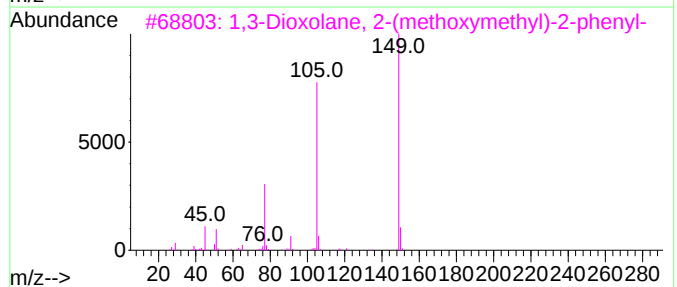
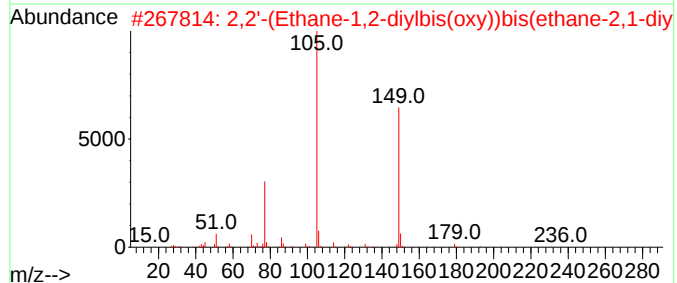
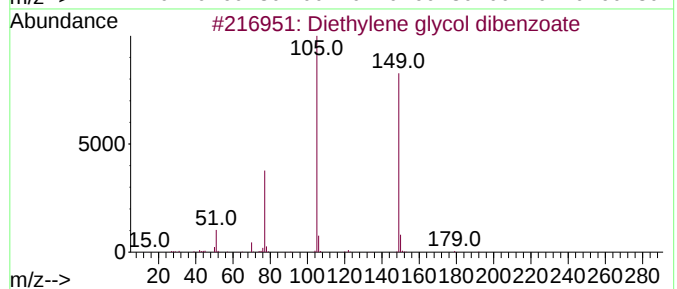
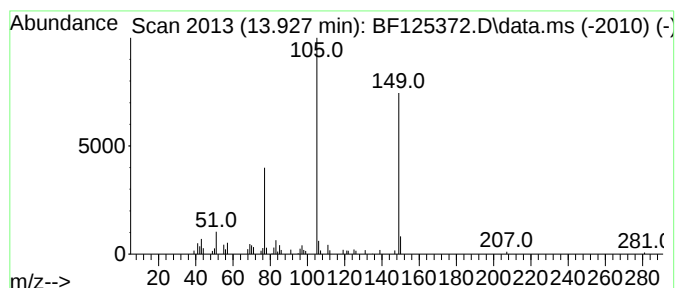
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Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.927	2.65 ng	105480	Chrysene-d12	14.062	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	78
2	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	72
3	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59
4	Phthalic acid, isohexyl 2-pentyl...	320	C19H28O4	1000315-48-7	38
5	Phthalic acid, cyclobutyl decyl ...	360	C22H32O4	1000314-90-5	38



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.193	97.1	ng	4143780	1	6.898	853590	20.0
Ethanol, 2-(2-b...	8.080	3.3	ng	175099	2	8.180	1057040	20.0
1,2-Benzenedica...	11.580	20.2	ng	1031090	4	11.421	1020210	20.0
n-Hexadecanoic ...	11.939	3.4	ng	172815	4	11.421	1020210	20.0
Diethylene glyc...	13.927	2.6	ng	105480	5	14.062	796524	20.0