

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091321\
 Data File : BF125454.D
 Acq On : 13 Sep 2021 20:48
 Operator : JU/CG
 Sample : M3684-07
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A019015

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: BF125454.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	24	rBV	985675	1287893	37.87%	5.165%
2	2.299	32	36	43	rVB	48871	65411	1.92%	0.262%
3	5.110	510	514	524	rVB	165262	192289	5.65%	0.771%
4	5.510	578	582	603	rBV	3026371	3087496	90.79%	12.381%
5	6.522	749	754	757	rBV	3110360	3014114	88.63%	12.087%
6	6.887	812	816	819	rBV	1019454	902745	26.55%	3.620%
7	7.451	907	912	915	rBV	2122619	1990326	58.53%	7.982%
8	8.081	1013	1019	1030	rBV	92890	272099	8.00%	1.091%
9	8.169	1030	1034	1048	rVB	1410122	1218231	35.82%	4.885%
10	9.245	1212	1217	1220	rBV	4056693	3400673	100.00%	13.637%
11	9.928	1329	1333	1336	rBV	1529838	1271466	37.39%	5.099%
12	10.716	1463	1467	1476	rBV	2333805	2123719	62.45%	8.517%
13	11.416	1582	1586	1589	rBV	1453163	1192085	35.05%	4.780%
14	11.933	1670	1674	1684	rBV2	123620	134080	3.94%	0.538%
15	12.504	1763	1771	1776	rBV4	30779	39820	1.17%	0.160%
16	12.721	1801	1808	1813	rBV4	67484	78871	2.32%	0.316%
17	12.863	1829	1832	1836	rVB	60101	53797	1.58%	0.216%
18	13.004	1851	1856	1859	rBV	3078957	2707355	79.61%	10.857%
19	13.963	2012	2019	2022	rBV7	37911	89859	2.64%	0.360%
20	14.063	2032	2036	2044	rVB	931917	882644	25.95%	3.540%
21	14.210	2058	2061	2066	rBV2	41897	42378	1.25%	0.170%
22	15.557	2285	2290	2297	rBV2	682354	889060	26.14%	3.565%

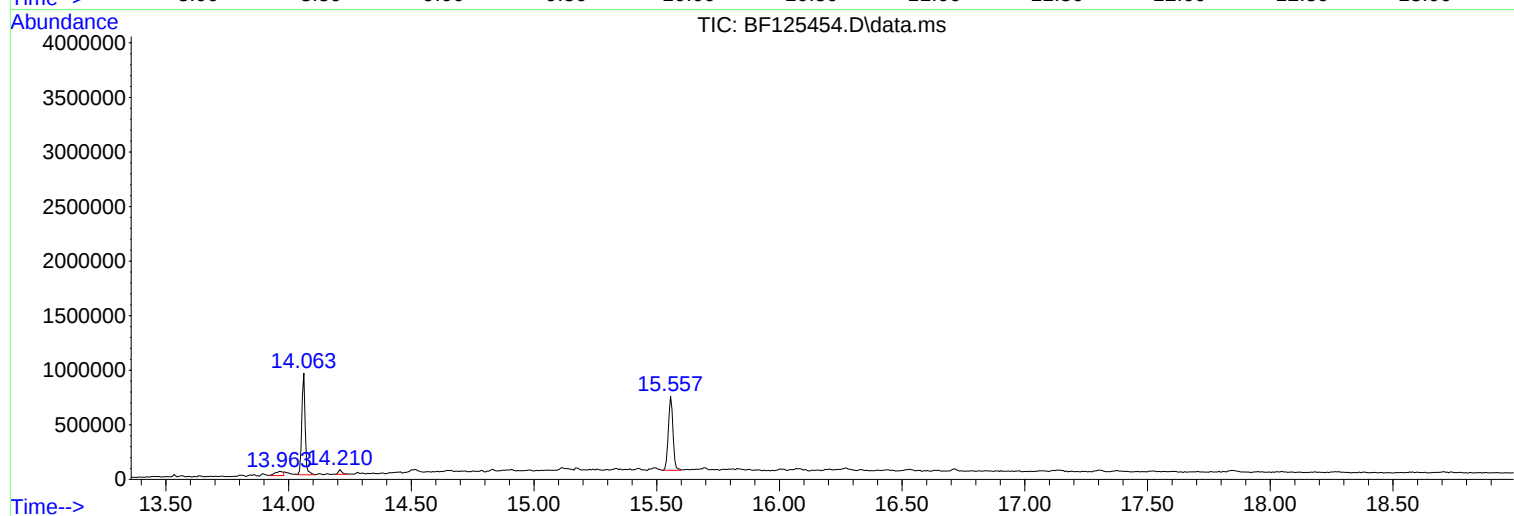
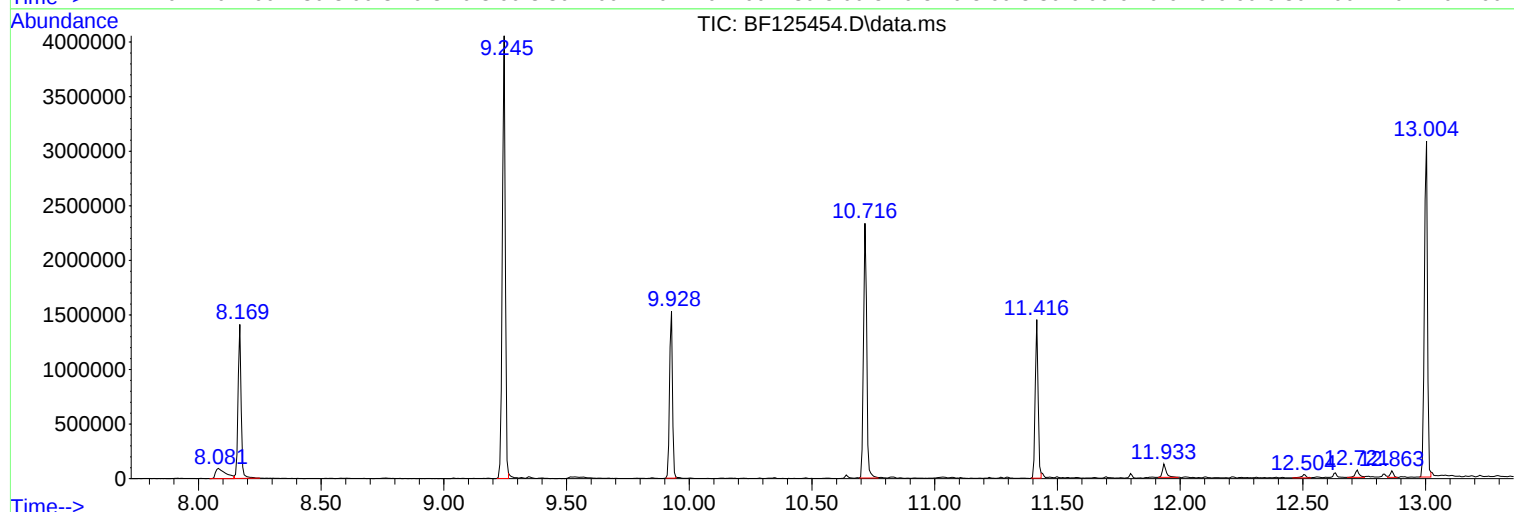
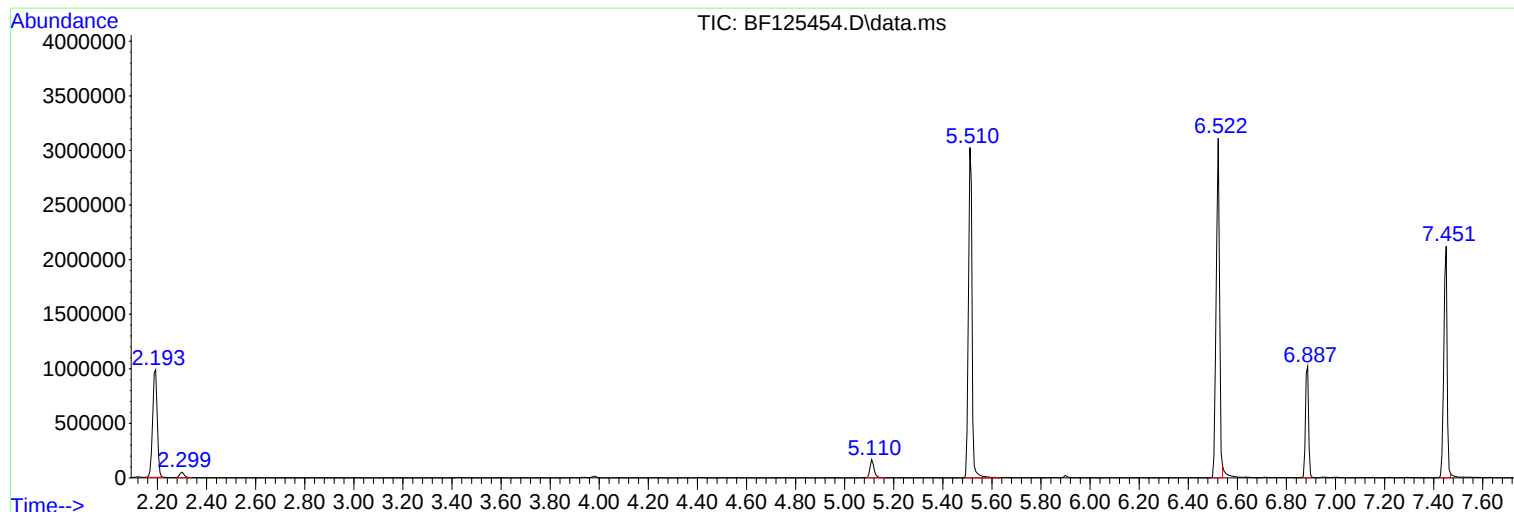
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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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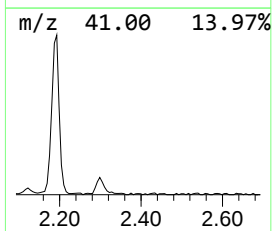
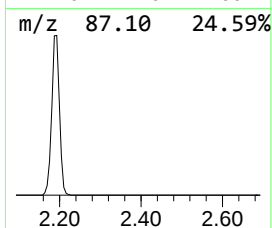
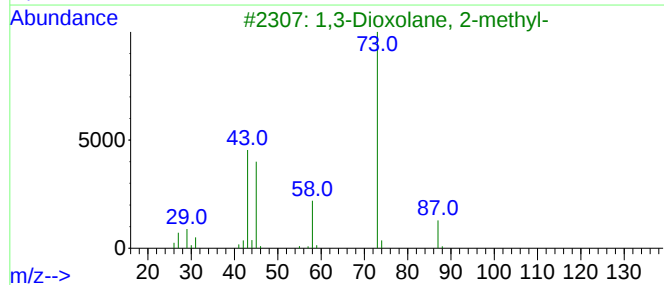
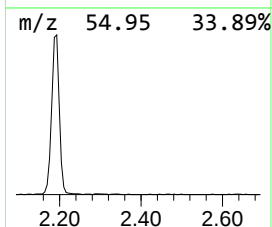
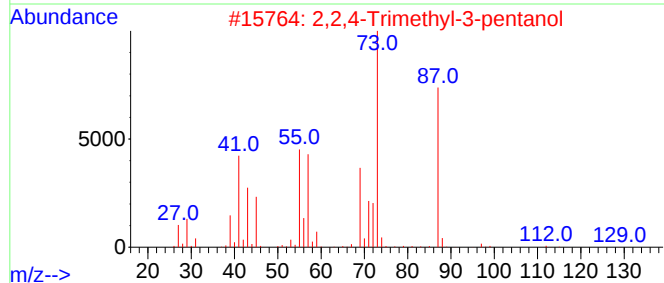
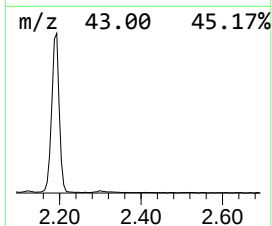
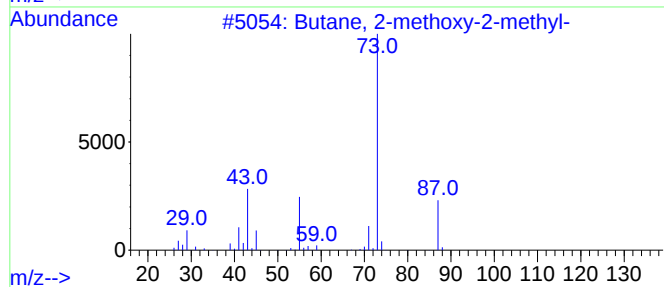
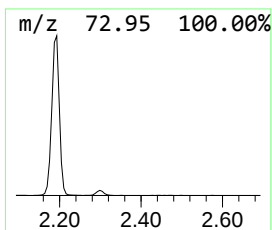
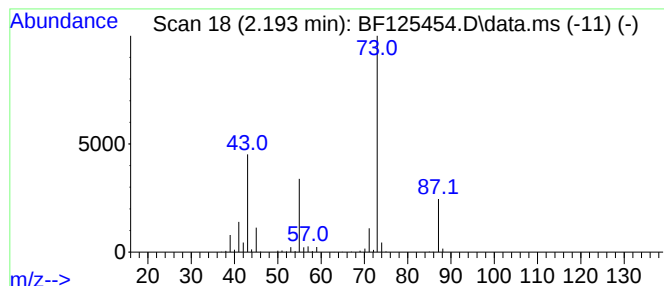
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	28.53 ng	1287890	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23



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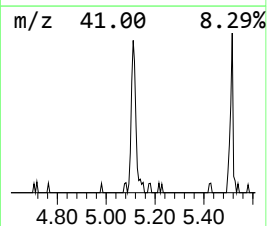
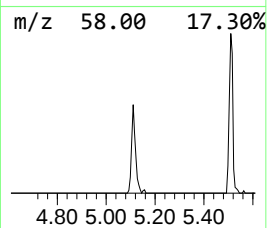
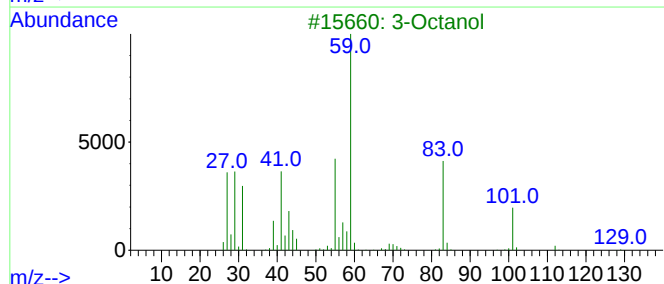
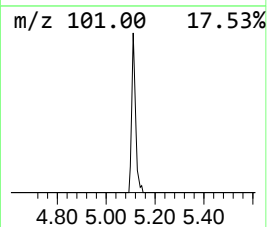
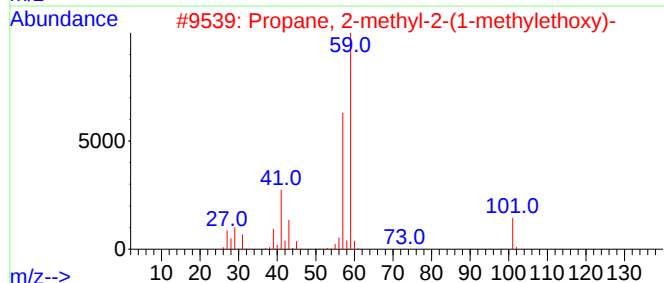
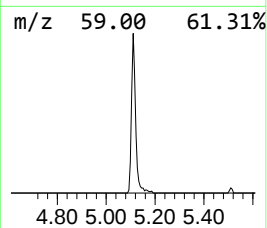
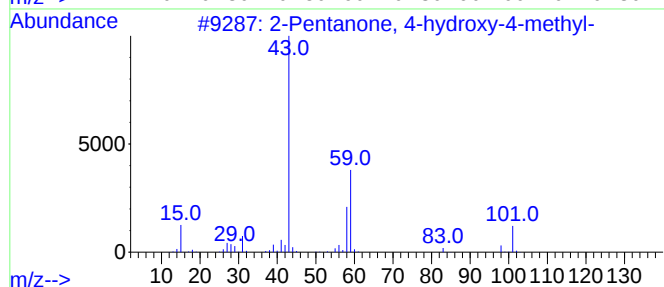
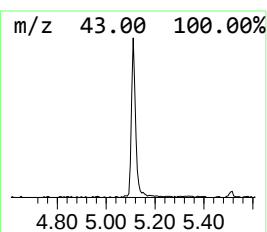
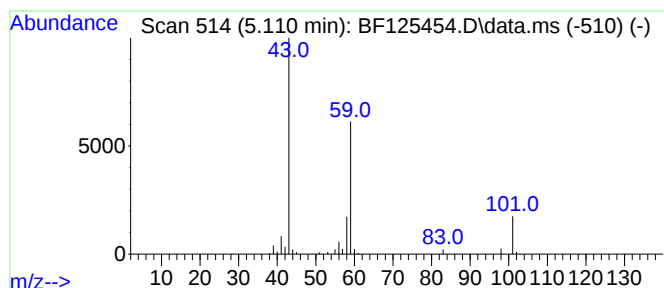
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	4.26 ng	192289	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Octanol	130	C8H18O	000589-98-0	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33



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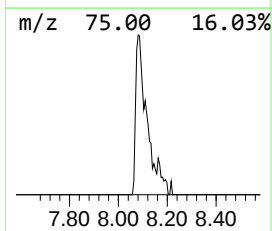
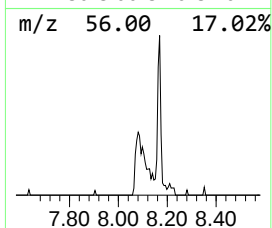
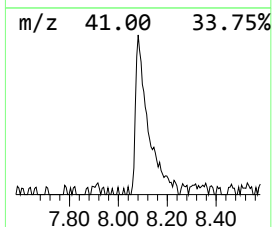
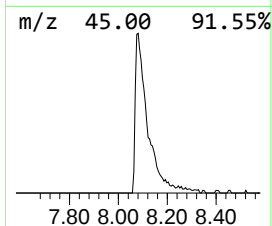
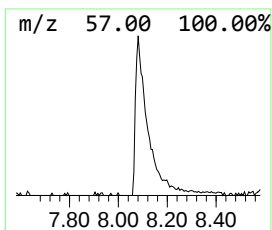
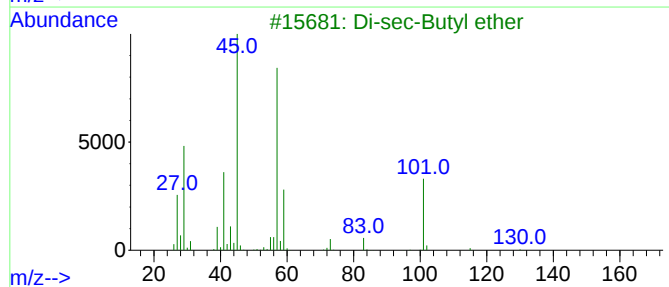
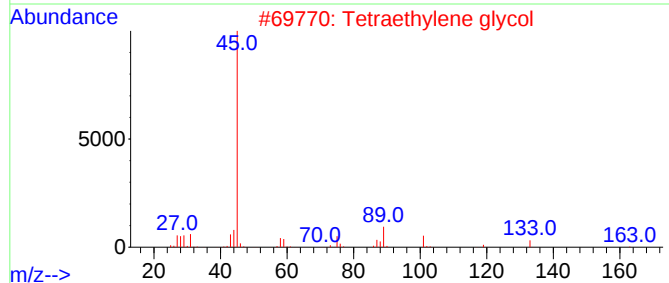
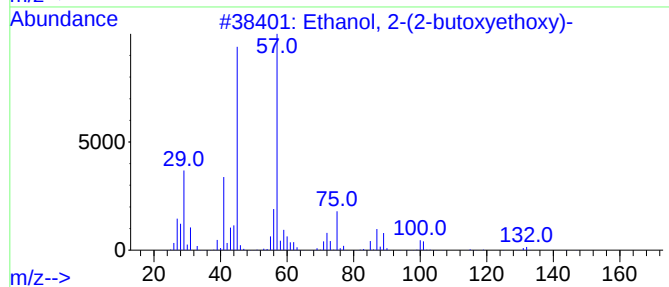
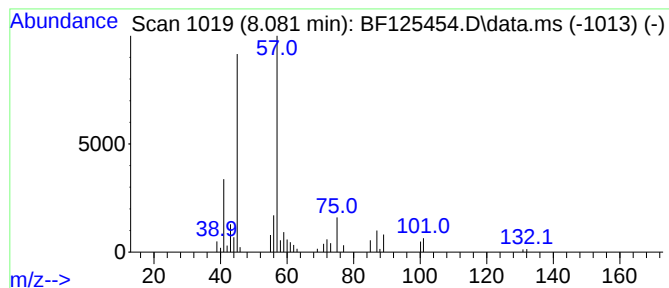
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.081	4.47 ng	272099	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Tetraethylene glycol	194	C8H18O5	000112-60-7	59
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
5			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50



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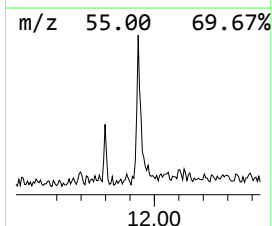
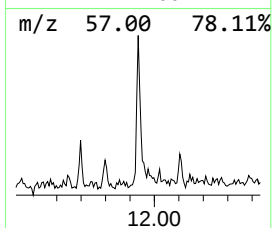
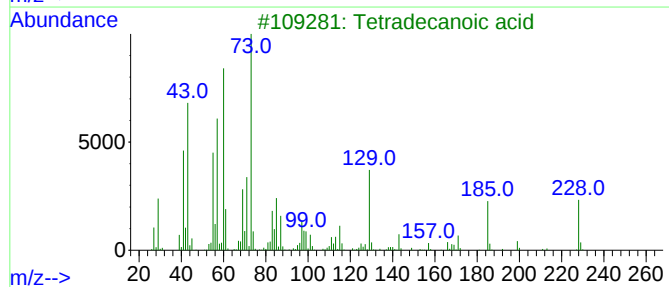
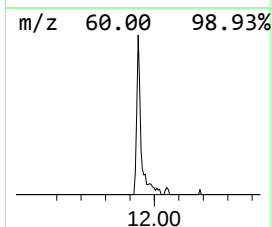
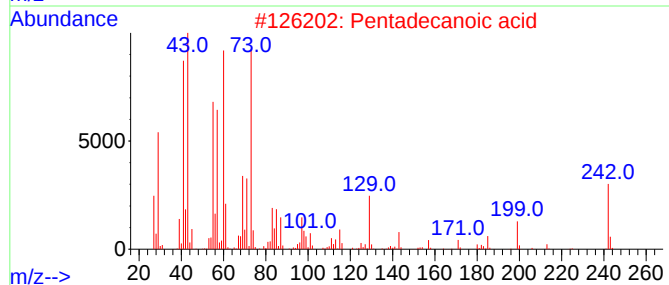
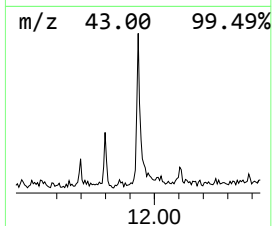
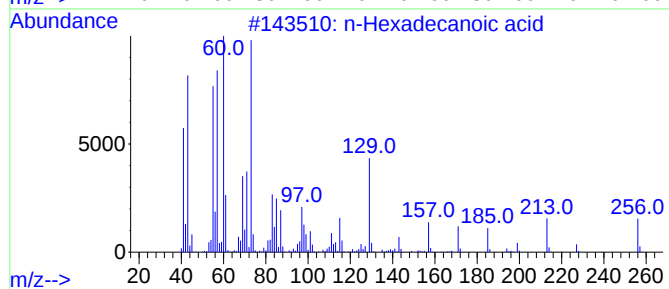
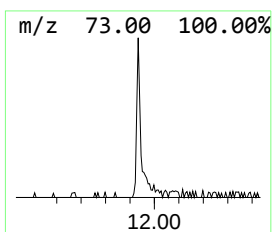
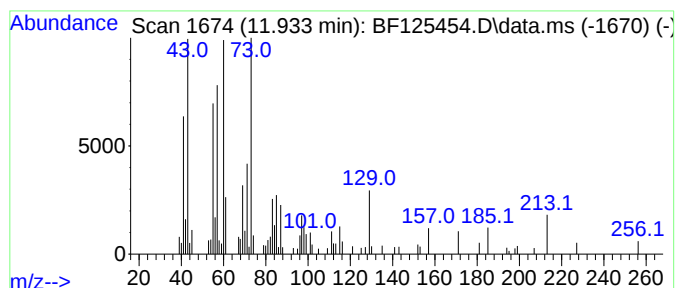
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	2.25 ng	134080	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			Tetradecane	198	C14H30	000629-59-4	25



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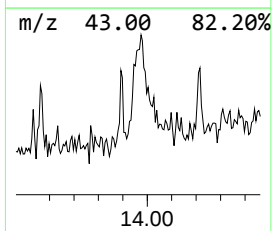
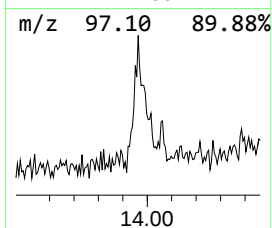
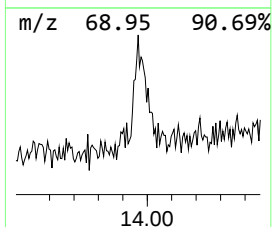
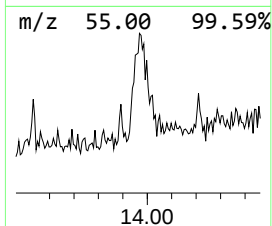
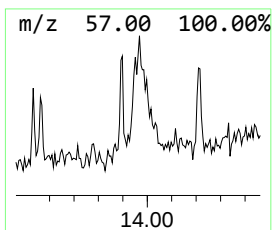
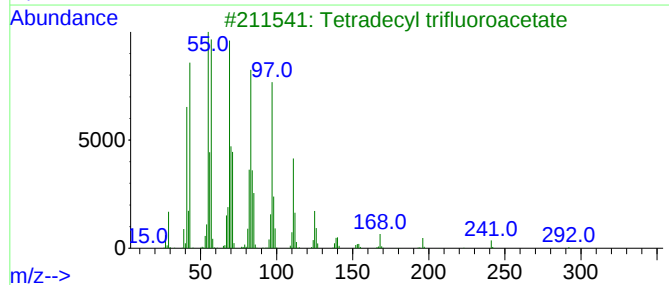
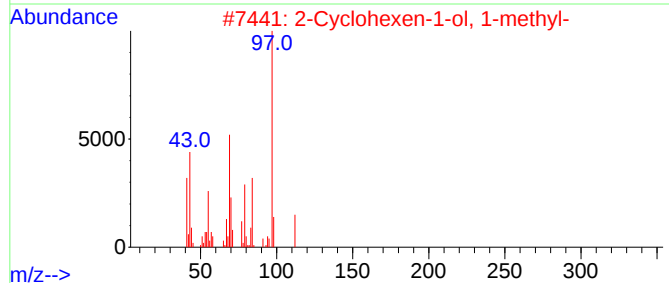
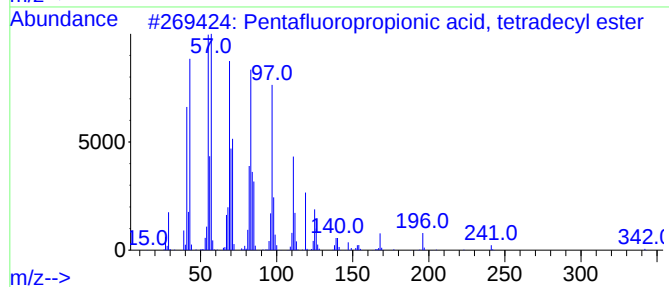
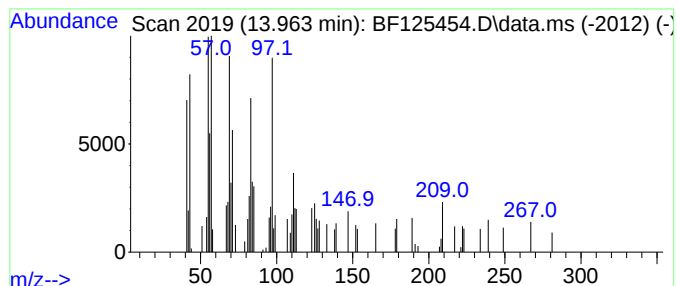
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.963	2.04 ng	89859	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	64
2			2-Cyclohexen-1-ol, 1-methyl-	112	C7H12O	023758-27-2	60
3			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	58
4			n-Nonadecanol-1	284	C19H40O	001454-84-8	52
5			Chloroacetic acid, tridecyl ester	276	C15H29ClO2	018277-85-5	52



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.193	28.5	ng	1287890	1	6.887	902745	20.0
2-Pentanone, 4-...	5.110	4.3	ng	192289	1	6.887	902745	20.0
Ethanol, 2-(2-b...	8.081	4.5	ng	272099	2	8.169	1218230	20.0
n-Hexadecanoic ...	11.933	2.3	ng	134080	4	11.416	1192090	20.0
Pentafluoroprop...	13.963	2.0	ng	89859	5	14.063	882644	20.0