

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
 Data File : BF125207.D
 Acq On : 25 Aug 2021 13:42
 Operator : JU/CG
 Sample : M3524-02
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PE-2

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: BF125207.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	14	20	27	rVB	800430	1034352	28.91%	3.995%
2	5.528	581	585	589	rBV	3051786	3080846	86.10%	11.900%
3	6.534	751	756	759	rBV	2971392	3133925	87.59%	12.105%
4	6.916	817	821	824	rBV	1001273	877526	24.52%	3.390%
5	7.475	911	916	919	rBV	2375276	2053425	57.39%	7.932%
6	8.092	1018	1021	1035	rBV	86900	197735	5.53%	0.764%
7	8.198	1035	1039	1042	rBV	1280060	1139170	31.84%	4.400%
8	9.269	1217	1221	1224	rBV	4140600	3578096	100.00%	13.821%
9	9.951	1333	1337	1340	rBV	1590090	1272126	35.55%	4.914%
10	10.739	1467	1471	1474	rBV	2774856	2410888	67.38%	9.312%
11	11.439	1586	1590	1593	rBV	1553137	1300863	36.36%	5.025%
12	11.957	1674	1678	1683	rBV	166091	175816	4.91%	0.679%
13	12.739	1808	1811	1820	rBV	61182	69406	1.94%	0.268%
14	13.022	1855	1859	1863	rBV	3578713	3433384	95.96%	13.262%
15	13.874	2000	2004	2007	rBV	31675	41379	1.16%	0.160%
16	13.910	2007	2010	2013	rBV	46913	51720	1.45%	0.200%
17	13.945	2013	2016	2019	rBV	118022	117193	3.28%	0.453%
18	13.998	2019	2025	2035	rVV8	41444	142768	3.99%	0.551%
19	14.074	2035	2038	2042	rVB	938426	884390	24.72%	3.416%
20	15.574	2287	2293	2303	rVB	738697	894318	24.99%	3.454%

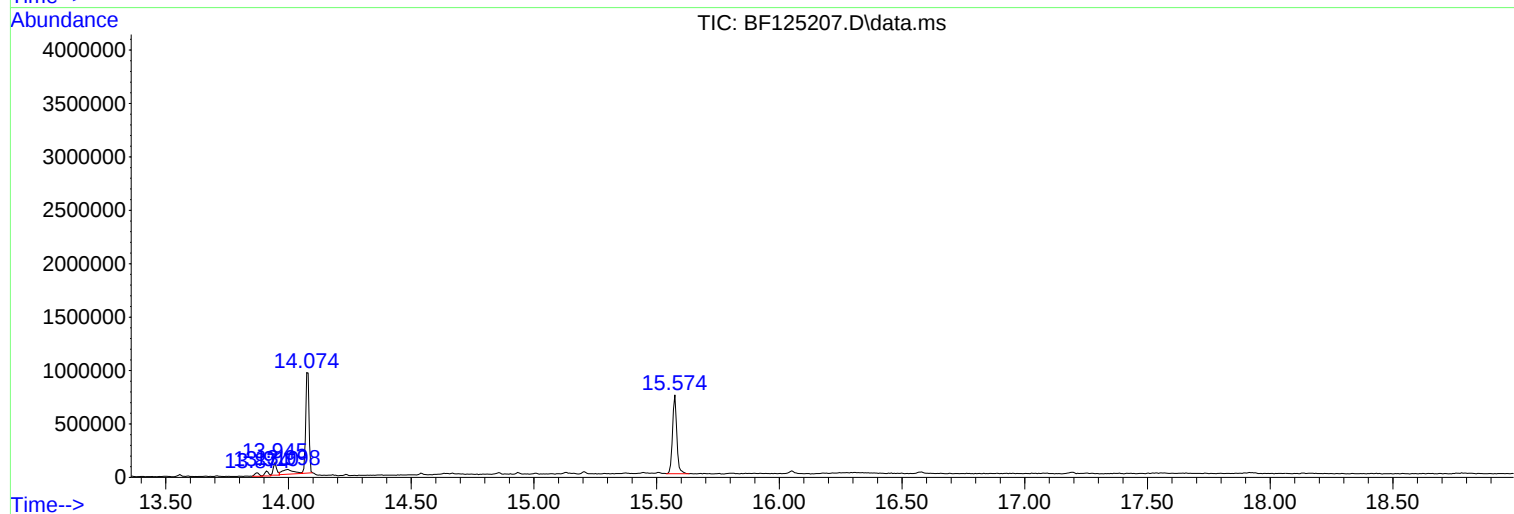
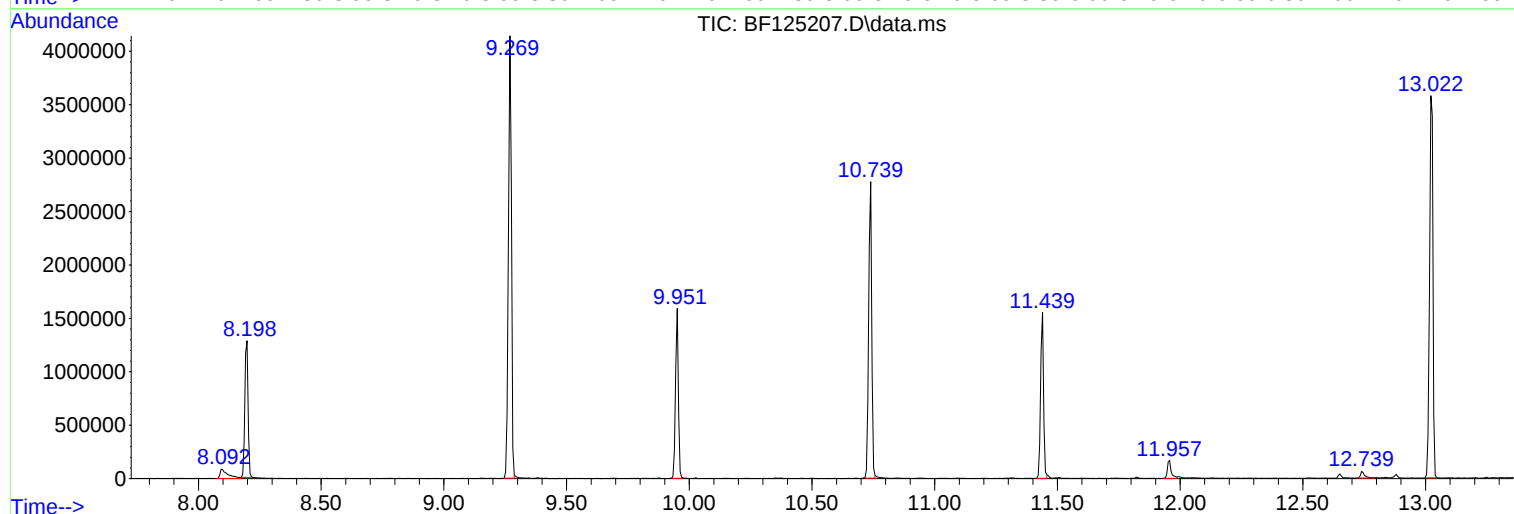
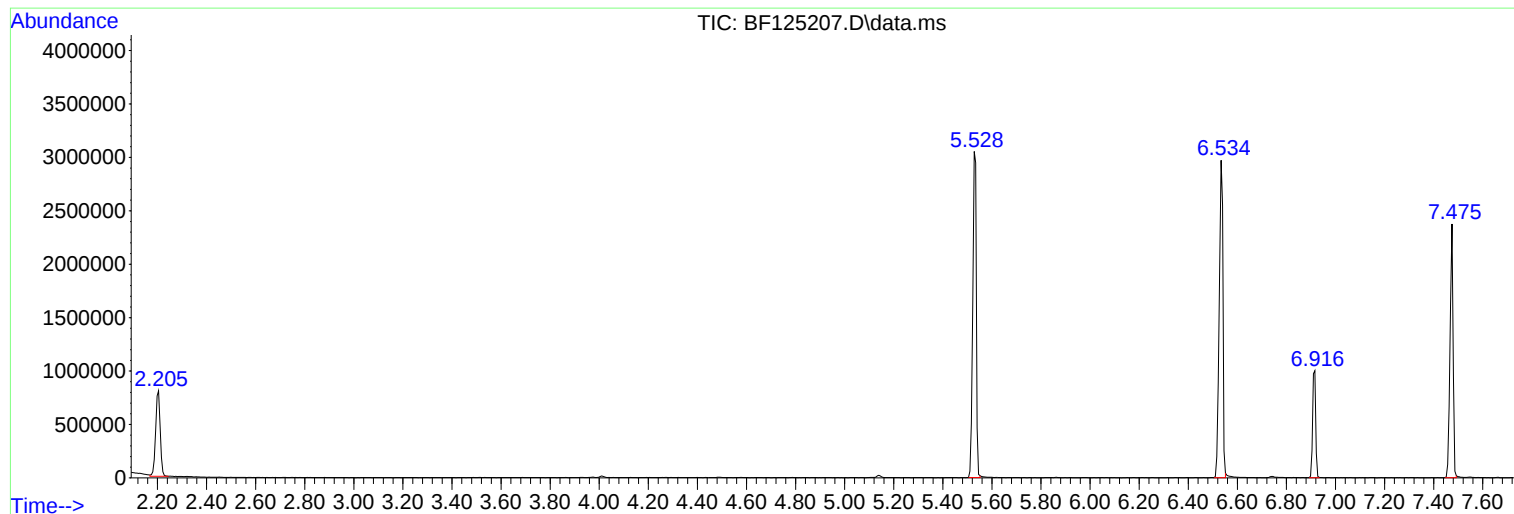
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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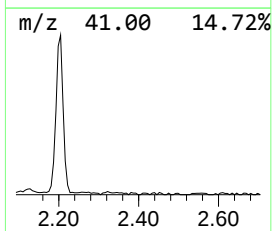
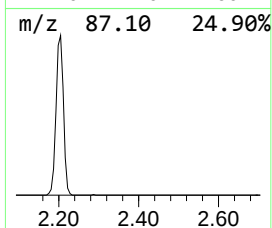
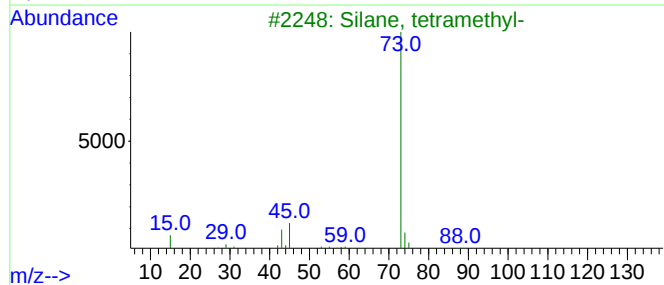
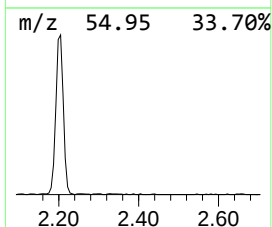
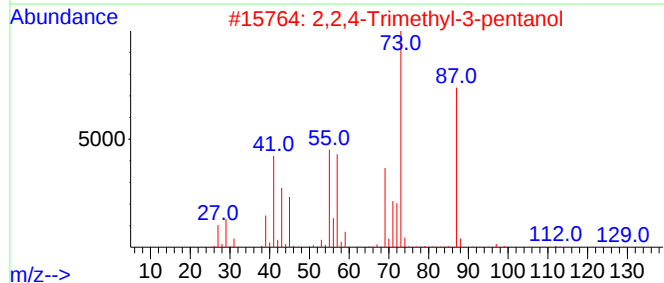
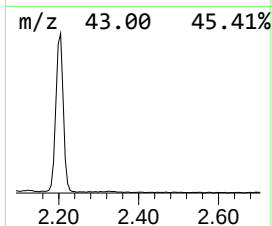
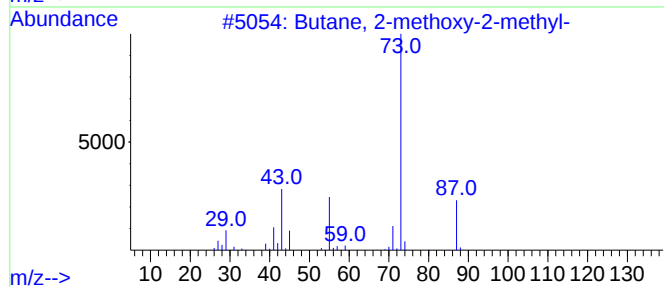
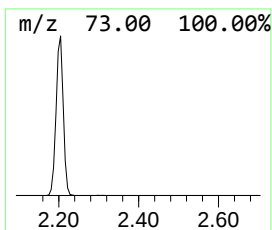
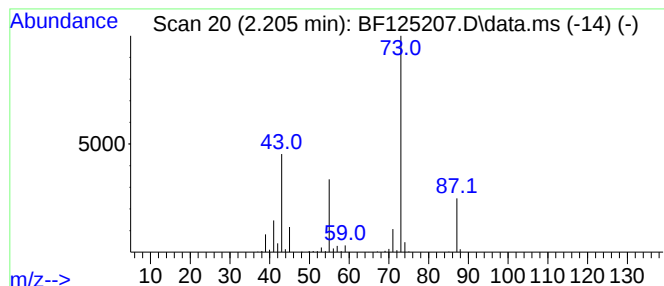
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.205	23.57 ng	1034350	1,4-Dichlorobenzene-d4	6.916

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	38
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	23
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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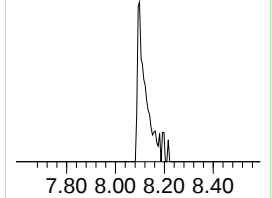
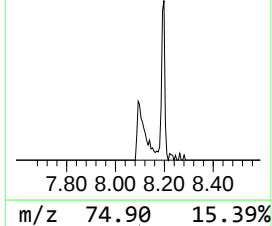
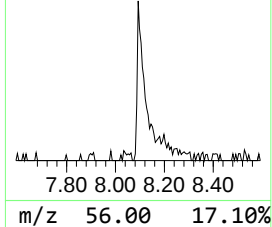
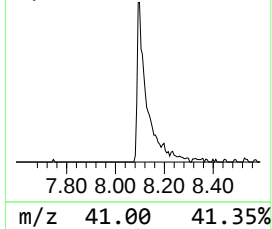
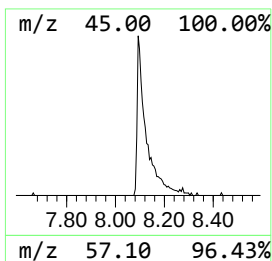
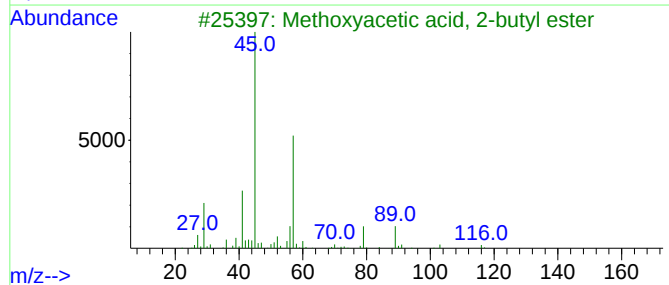
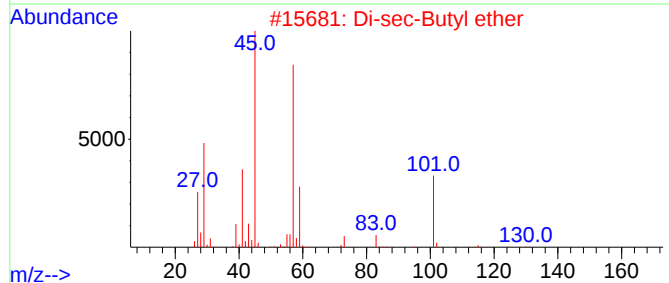
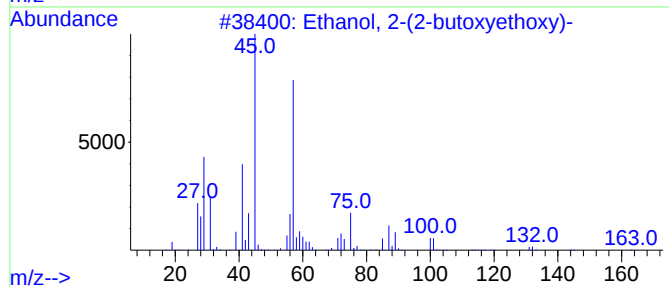
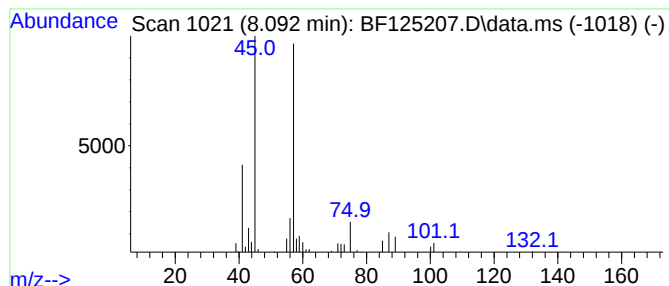
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	3.47 ng	197735	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2			Di-sec-Butyl ether	130	C8H18O	006863-58-7	59
3			Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	53
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50



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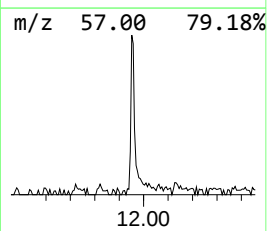
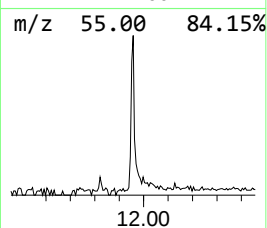
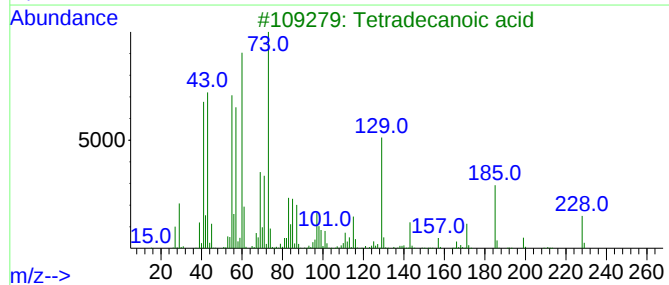
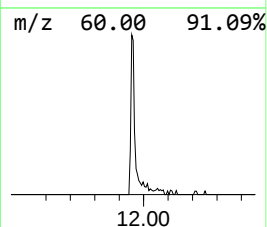
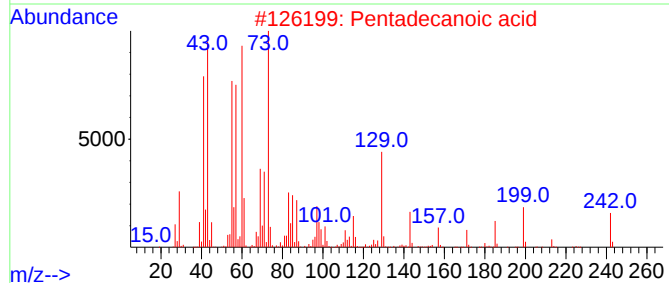
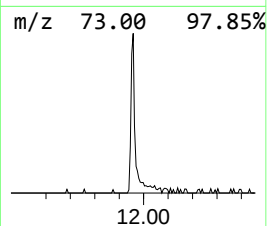
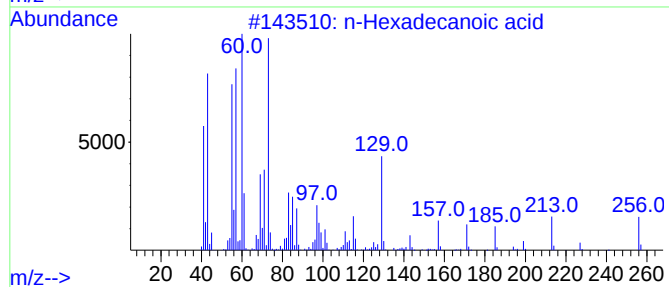
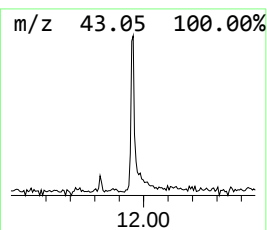
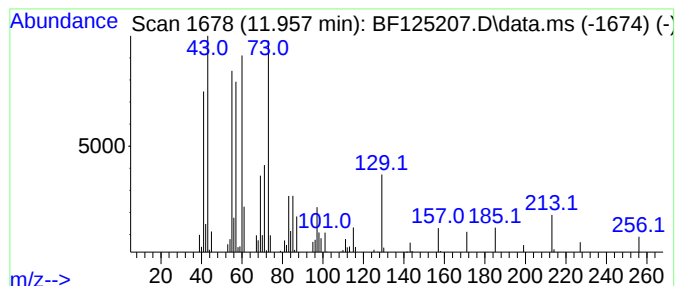
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	2.70 ng	175816	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Octanoic acid	144	C8H16O2	000124-07-2	50



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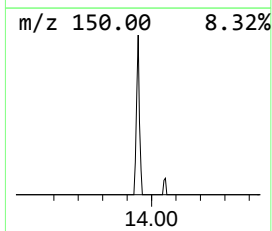
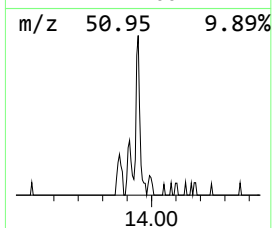
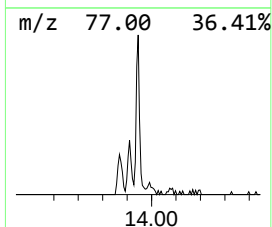
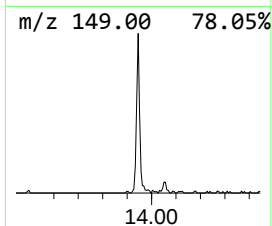
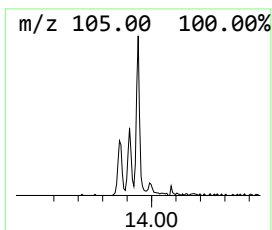
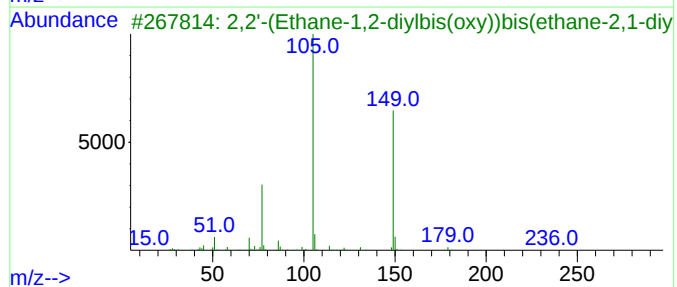
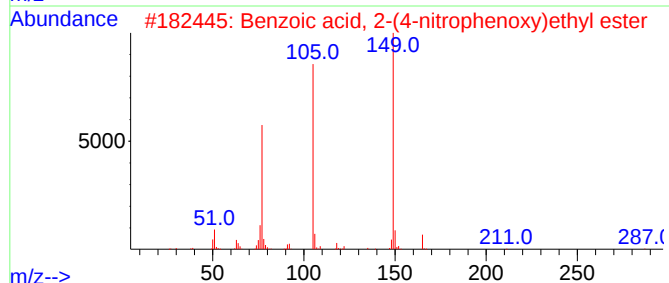
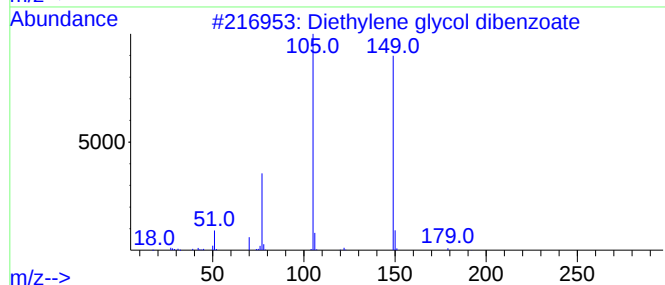
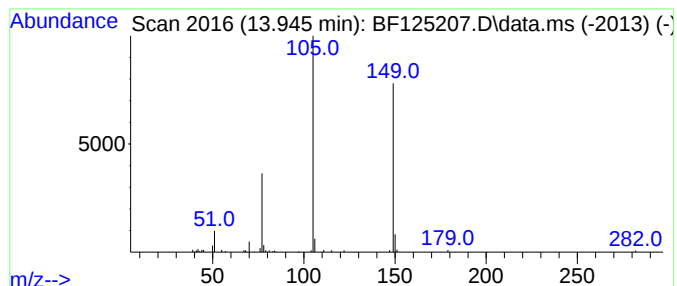
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.945	2.65 ng	117193	Chrysene-d12	14.080	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	72
3	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	64
4	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	64
5	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	50



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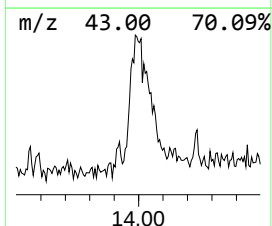
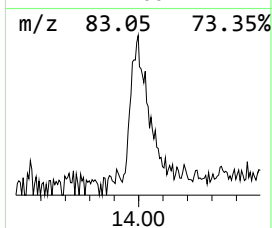
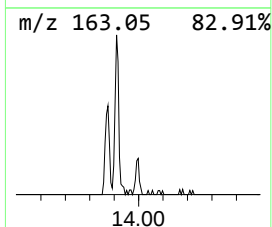
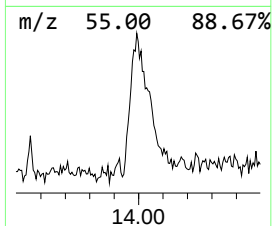
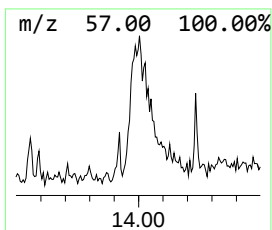
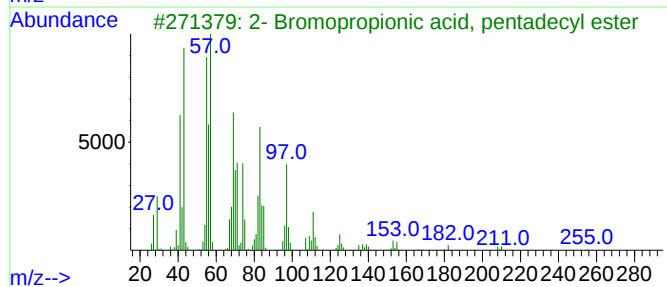
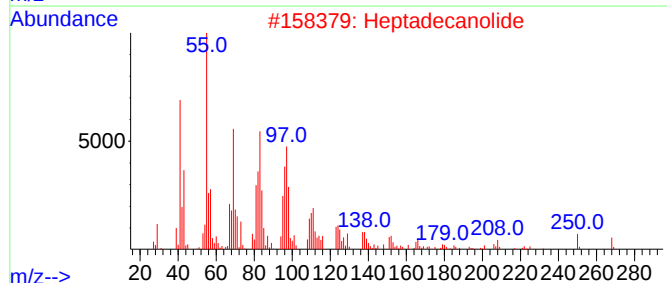
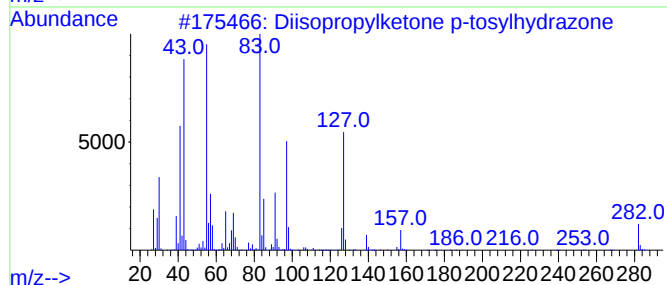
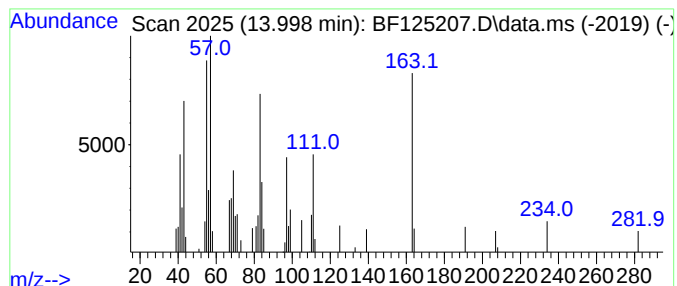
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown13.998 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	3.23 ng	142768	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diisopropylketone p-tosylhydrazone	282	C14H22N2O2S	017530-00-6	38
2			Heptadecanolide	268	C17H32O2	005637-97-8	35
3			2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	35
4			Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	35
5			Cyclohexanecarboxylic acid, 4-te...	324	C21H40O2	1000280-59-8	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.205	23.6	ng	1034350	1	6.916	877526	20.0
Ethanol, 2-(2-b...	8.092	3.5	ng	197735	2	8.198	1139170	20.0
n-Hexadecanoic ...	11.957	2.7	ng	175816	4	11.439	1300860	20.0
Diethylene glyc...	13.945	2.6	ng	117193	5	14.080	884390	20.0
unknown13.998	13.998	3.2	ng	142768	5	14.080	884390	20.0