

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
 Data File : BF125205.D
 Acq On : 25 Aug 2021 12:39
 Operator : JU/CG
 Sample : M3524-07
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PE-7

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: BF125205.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	26	rVB	879465	1119011	30.78%	4.167%
2	5.534	581	586	589	rBV	3209093	3173570	87.31%	11.817%
3	6.534	751	756	759	rBV	2963197	3211707	88.36%	11.959%
4	6.916	817	821	824	rBV	1024389	872814	24.01%	3.250%
5	7.475	911	916	919	rBV	2453026	2129282	58.58%	7.929%
6	8.098	1018	1022	1035	rBV	68179	156935	4.32%	0.584%
7	8.198	1035	1039	1042	rBV	1271830	1118241	30.76%	4.164%
8	9.269	1217	1221	1224	rBV	4231792	3634941	100.00%	13.535%
9	9.951	1333	1337	1340	rBV	1620809	1279026	35.19%	4.763%
10	10.739	1467	1471	1474	rBV	2954974	2543303	69.97%	9.470%
11	11.439	1586	1590	1593	rBV	1623088	1333882	36.70%	4.967%
12	11.957	1674	1678	1682	rBV	226946	237436	6.53%	0.884%
13	12.739	1808	1811	1824	rBV	71806	94118	2.59%	0.350%
14	13.021	1855	1859	1863	rVB	3702819	3617898	99.53%	13.472%
15	13.874	2000	2004	2007	rBV	36997	45931	1.26%	0.171%
16	13.910	2007	2010	2013	rBV	56510	54310	1.49%	0.202%
17	13.945	2013	2016	2018	rVV	147202	141234	3.89%	0.526%
18	13.992	2018	2024	2035	rVV8	72556	275679	7.58%	1.027%
19	14.080	2035	2039	2042	rVB	997483	955098	26.28%	3.556%
20	15.574	2288	2293	2304	rVB	700208	861056	23.69%	3.206%

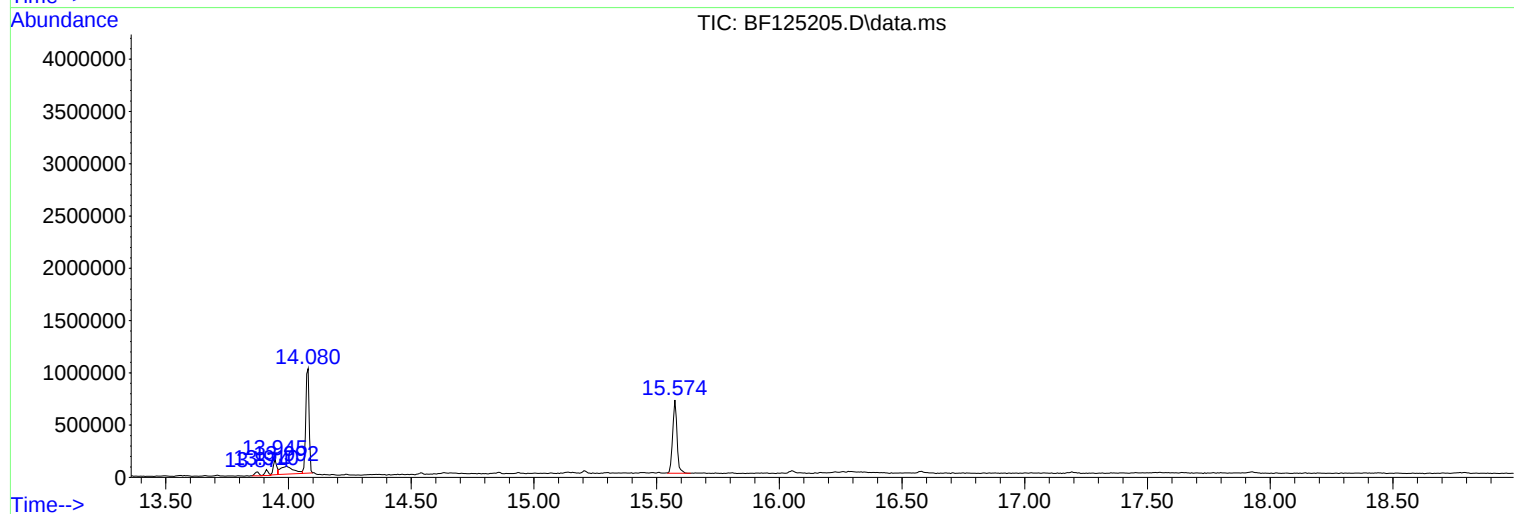
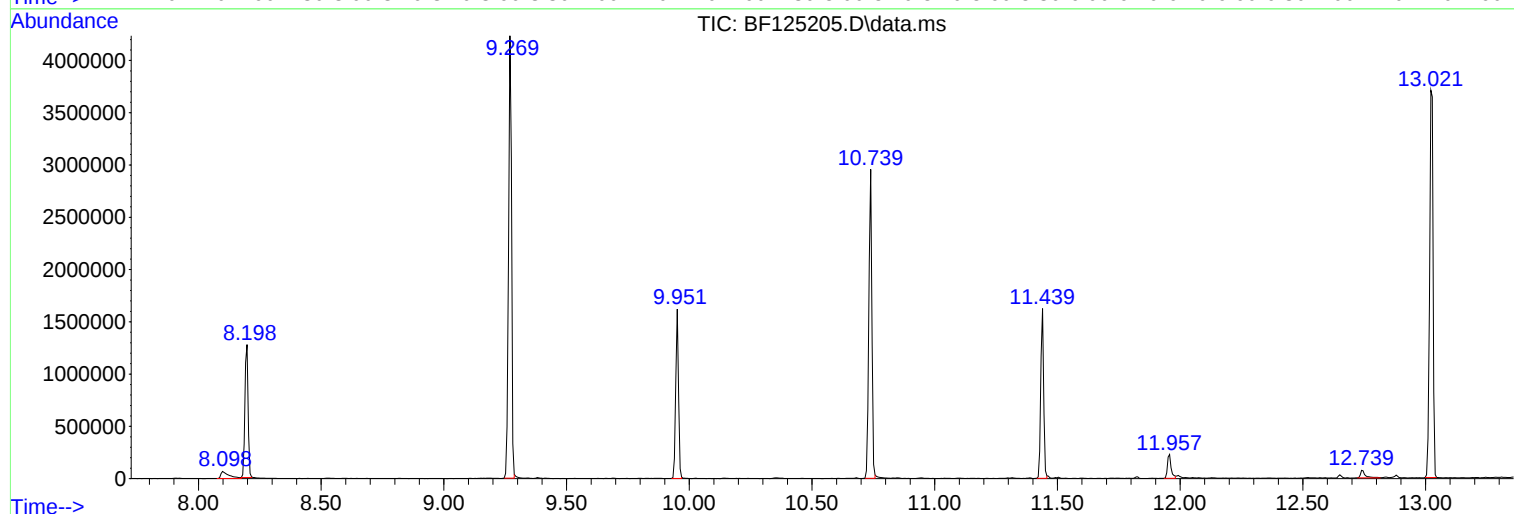
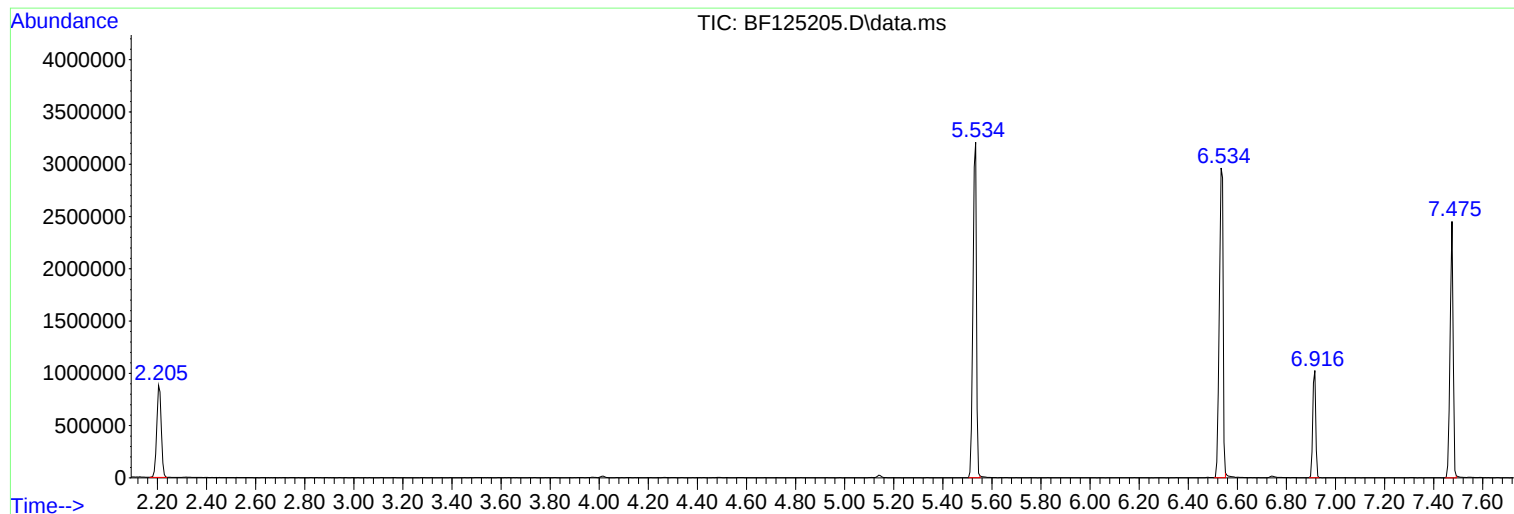
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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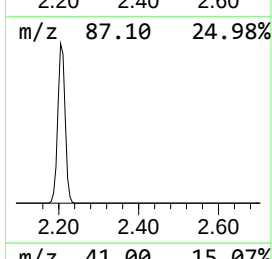
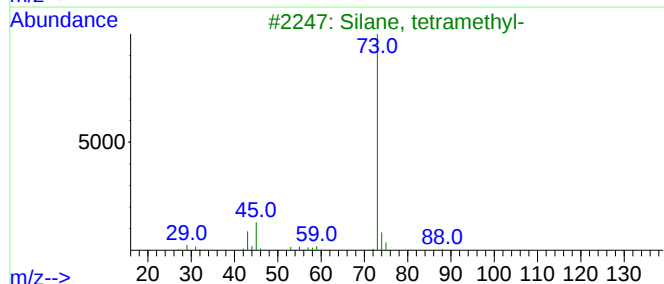
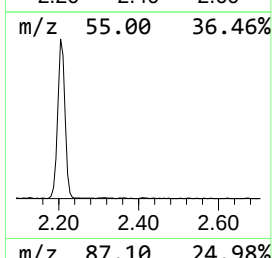
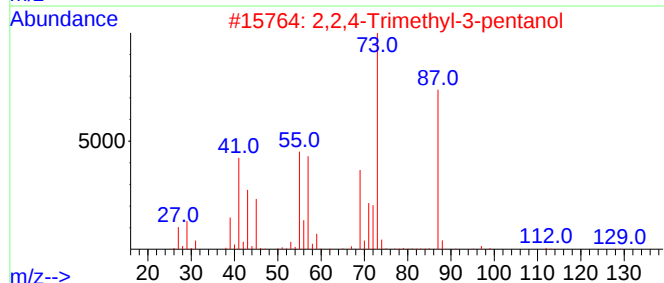
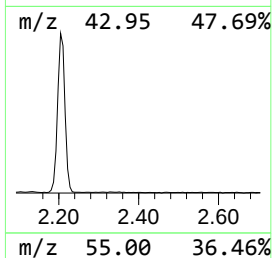
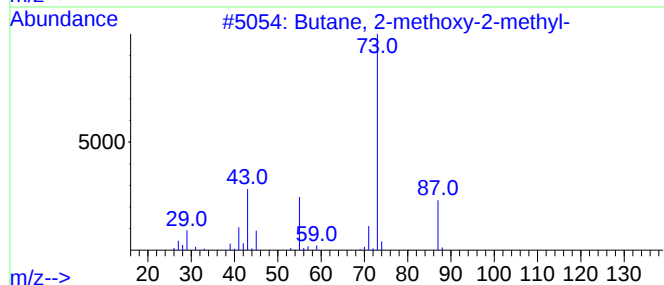
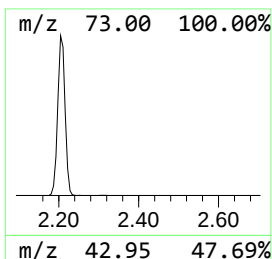
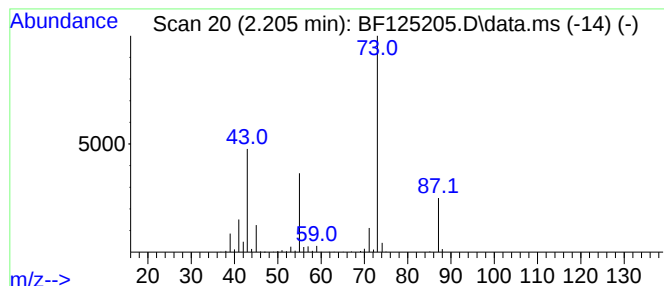
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.205	25.64 ng	1119010	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	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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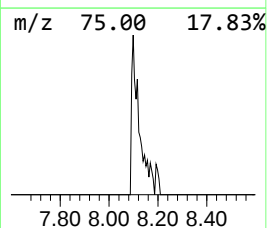
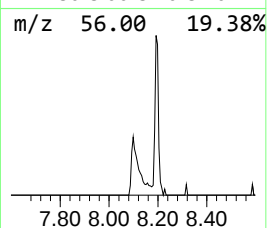
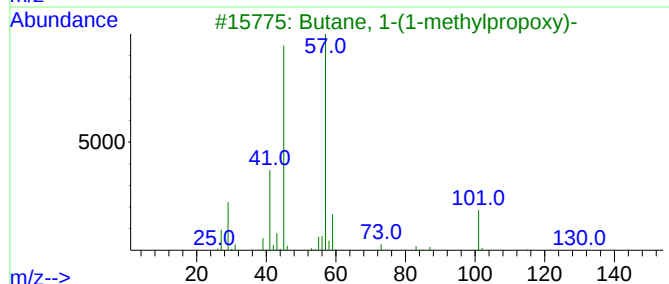
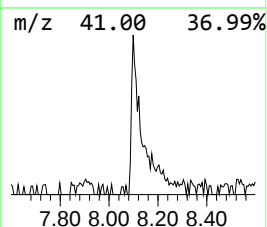
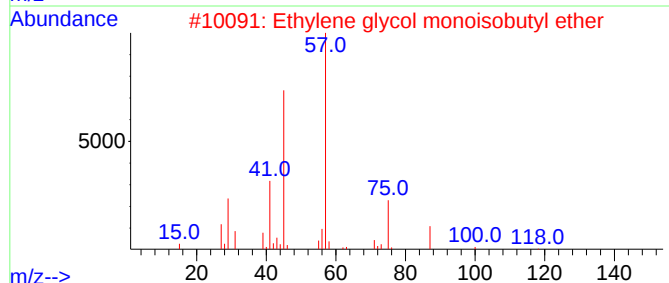
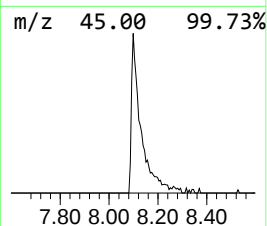
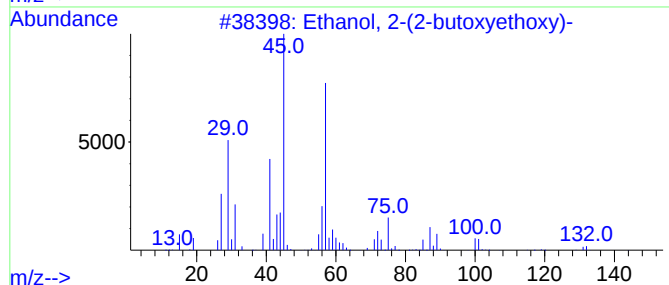
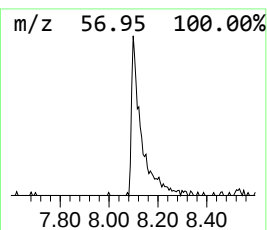
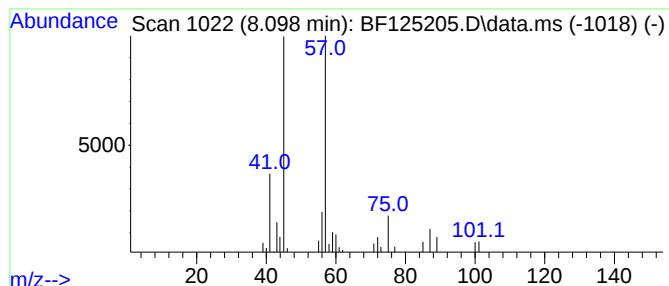
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	2.81 ng	156935	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
3			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5			Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	45



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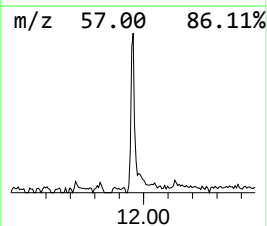
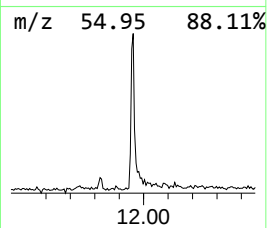
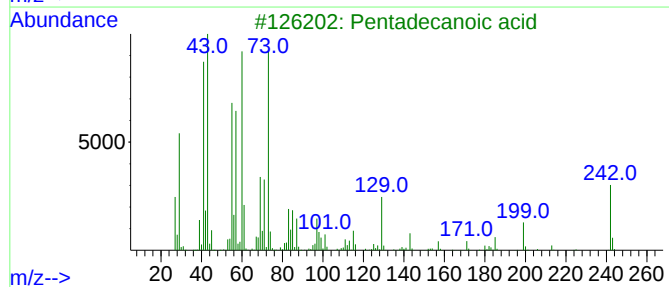
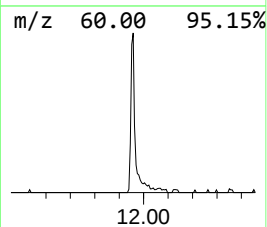
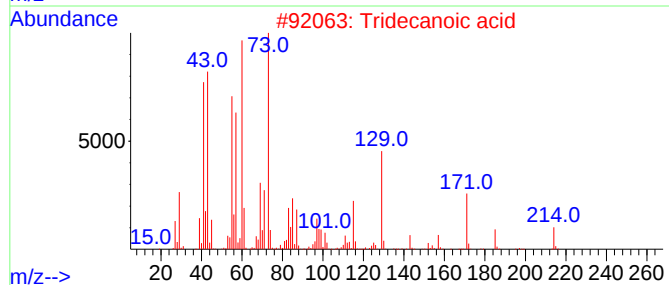
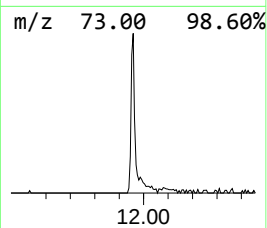
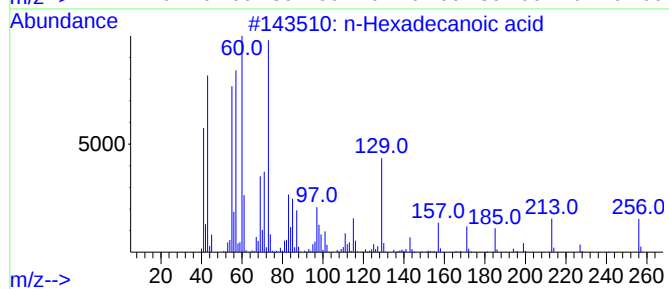
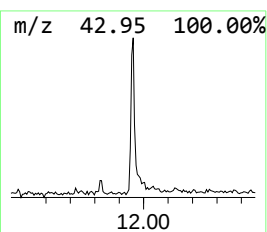
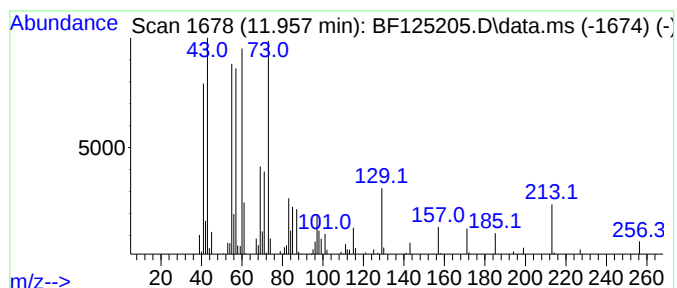
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	3.56 ng	237436	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	38



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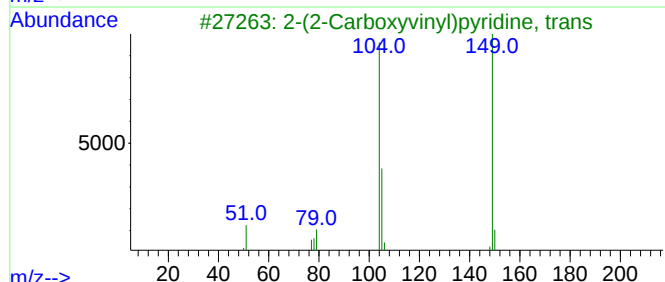
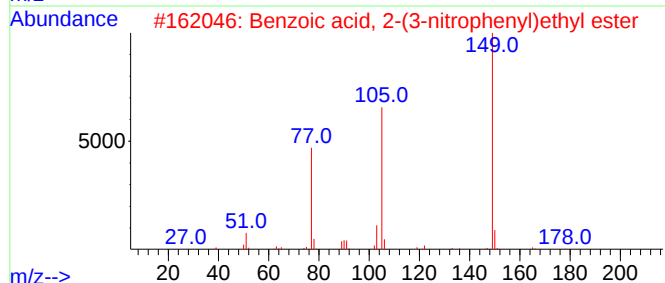
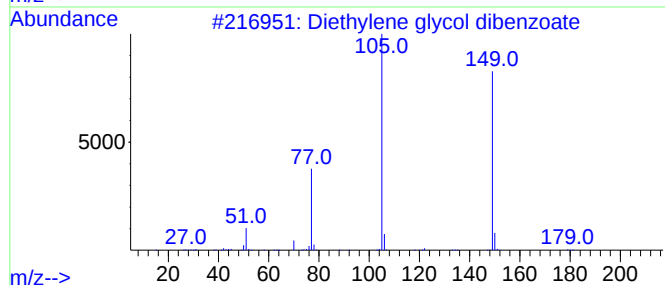
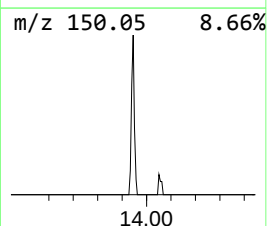
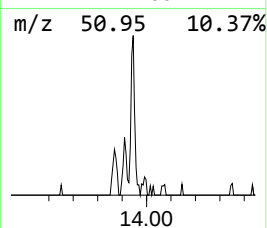
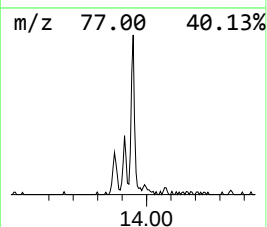
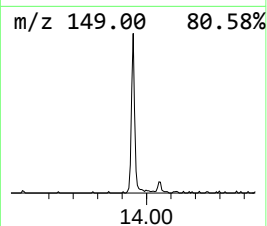
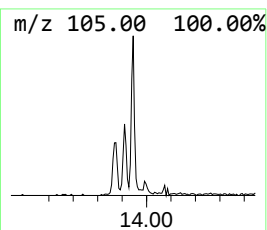
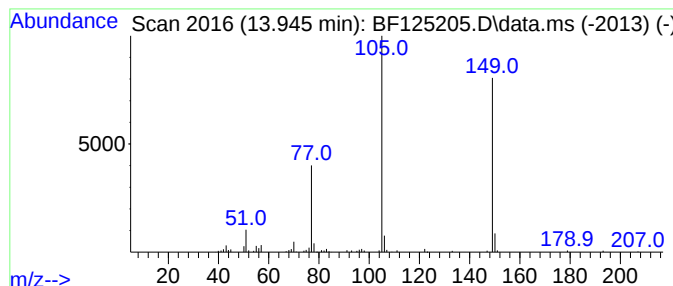
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Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	2.96 ng	141234	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-(3-nitrophenyl)ethyl ester	271	C15H13NO4	1000368-22-4	72
3			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	52
4			2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	43
5			Phthalic acid, hexyl heptyl ester	348	C21H32O4	1000308-93-8	38



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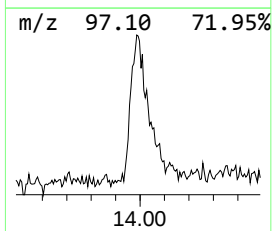
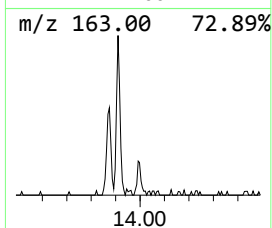
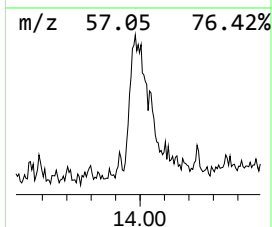
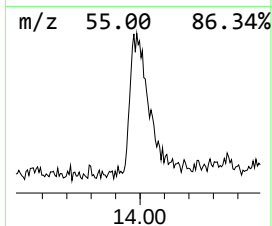
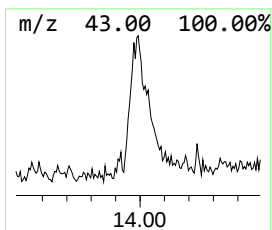
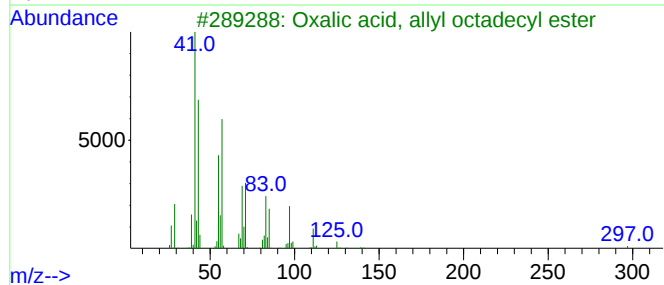
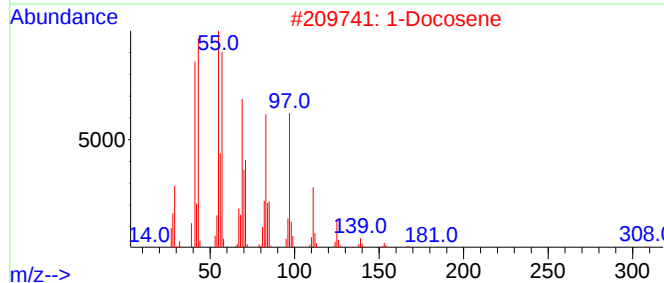
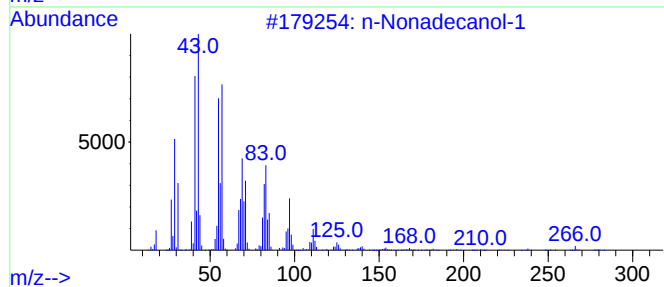
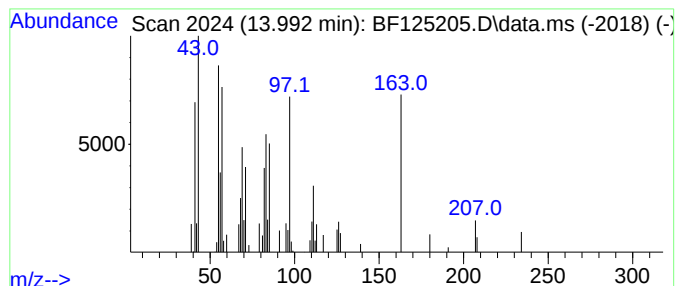
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Peak Number 5 unknown13.992 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.992	5.77 ng	275679	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Nonadecanol-1	284	C19H40O	001454-84-8	46
2			1-Docosene	308	C22H44	001599-67-3	43
3			Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	38
4			Cyclohexane, 1-(cyclohexylmethyl)...	208	C15H28	054934-95-1	35
5			Oxalic acid, cyclobutyl hexadecy...	368	C22H40O4	1000309-70-6	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.205	25.6	ng	1119010	1	6.916	872814	20.0
Ethanol, 2-(2-b...	8.098	2.8	ng	156935	2	8.198	1118240	20.0
n-Hexadecanoic ...	11.957	3.6	ng	237436	4	11.439	1333880	20.0
Diethylene glyc...	13.945	3.0	ng	141234	5	14.080	955098	20.0
unknown13.992	13.992	5.8	ng	275679	5	14.080	955098	20.0