

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071921\
 Data File : BF124620.D
 Acq On : 19 Jul 2021 18:42
 Operator : JU/CG
 Sample : M3083-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TT-087-RW7-IDWSO-20210715

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-BF070721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124620.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	23	27	30	rBB	7900	8903	4.02%	0.693%
2	5.528	581	585	588	rBB	136538	133178	60.16%	10.367%
3	6.528	750	755	758	rBB	126014	144393	65.22%	11.240%
4	6.910	817	820	823	rBB	47703	36725	16.59%	2.859%
5	7.475	911	916	919	rBB	101758	95062	42.94%	7.400%
6	8.092	1018	1021	1024	rBV	40998	33478	15.12%	2.606%
7	8.198	1035	1039	1042	rBB	56304	51926	23.46%	4.042%
8	9.275	1217	1222	1225	rBV	238575	199235	90.00%	15.510%
9	9.951	1334	1337	1340	rBB	71064	62068	28.04%	4.832%
10	10.745	1467	1472	1475	rBB	135574	123012	55.57%	9.576%
11	11.445	1587	1591	1594	rBB	76889	66788	30.17%	5.199%
12	11.963	1676	1679	1681	rBB	16198	11246	5.08%	0.875%
13	12.751	1810	1813	1815	rBB	5059	4022	1.82%	0.313%
14	13.033	1856	1861	1864	rBB	251698	221378	100.00%	17.234%
15	13.563	1947	1951	1954	rBB	18869	17881	8.08%	1.392%
16	14.080	2036	2039	2042	rBB	51144	43895	19.83%	3.417%
17	15.574	2289	2293	2297	rBB	28366	31389	14.18%	2.444%

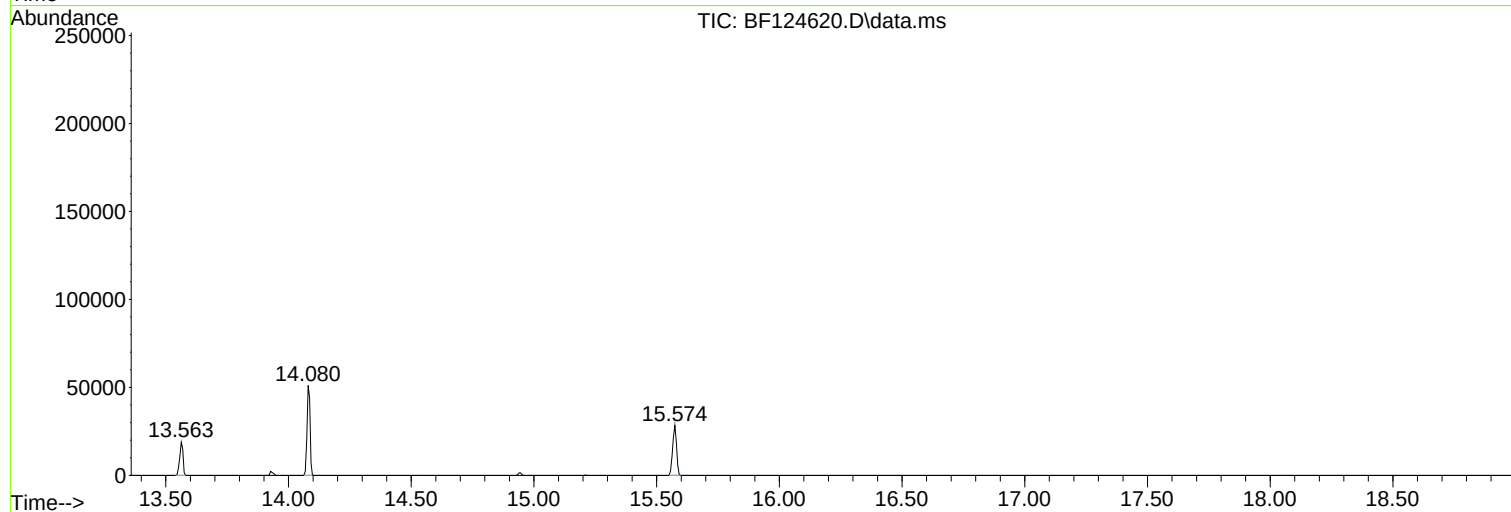
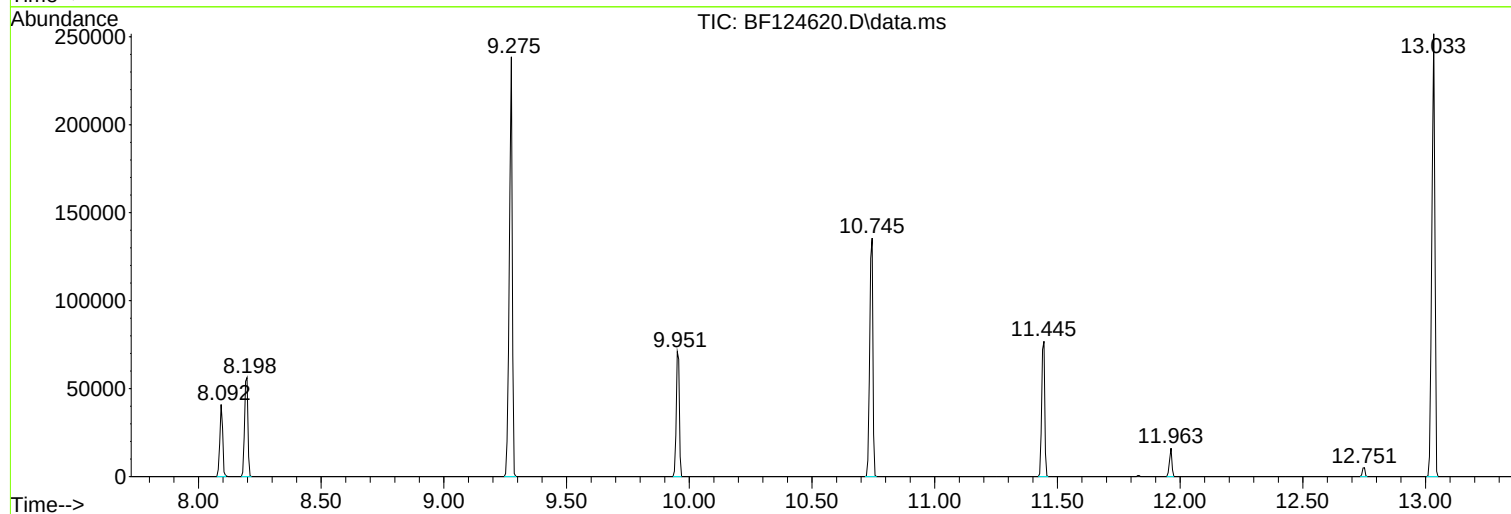
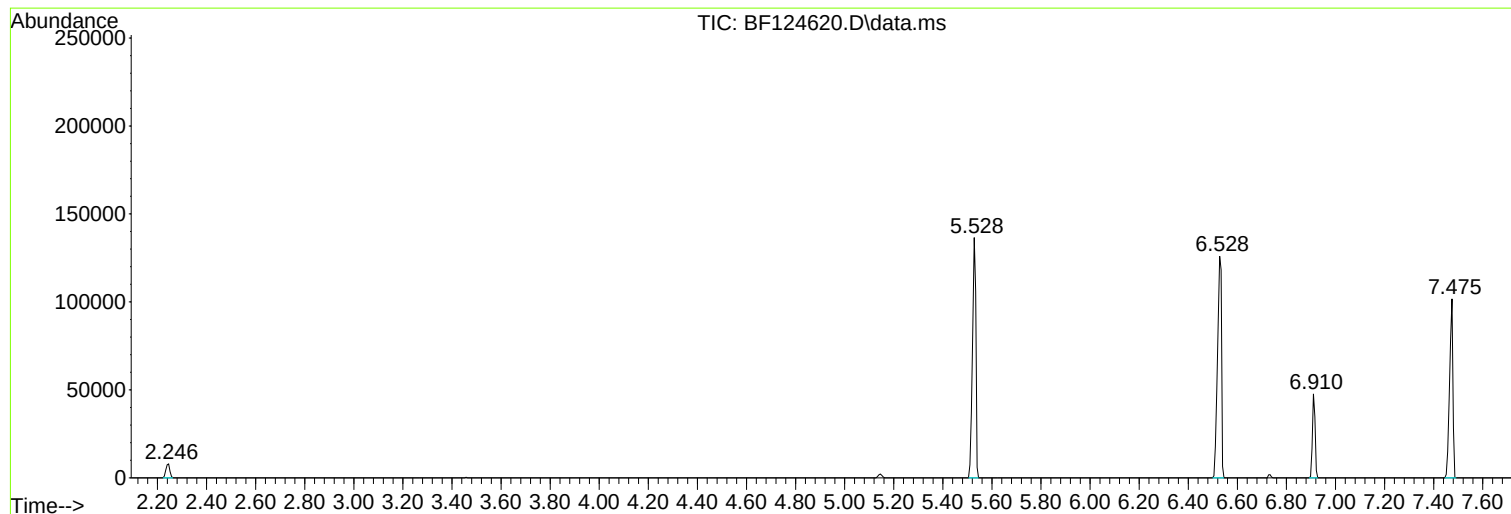
Sum of corrected areas: 1284579

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.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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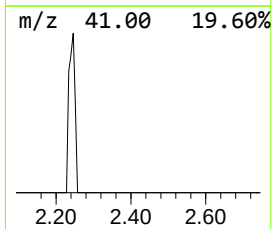
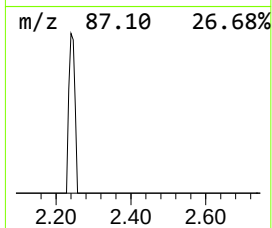
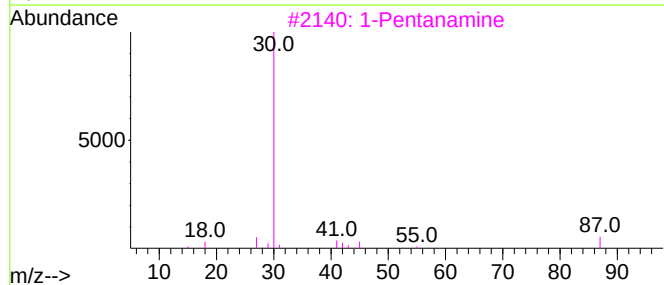
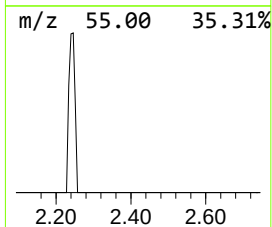
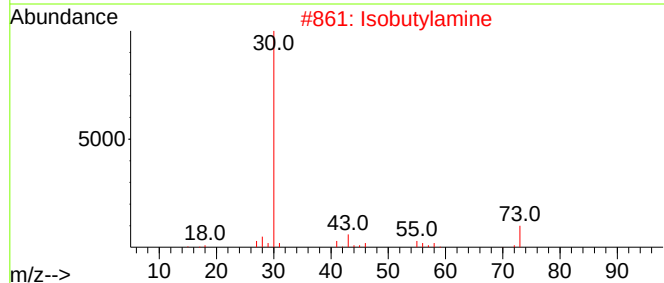
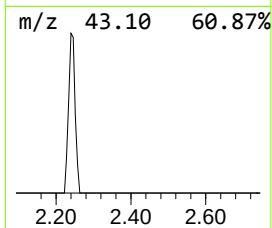
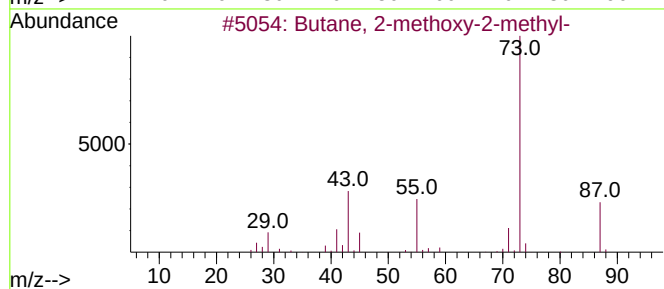
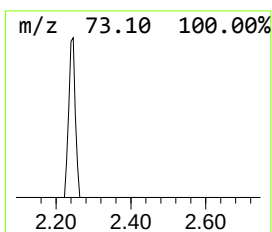
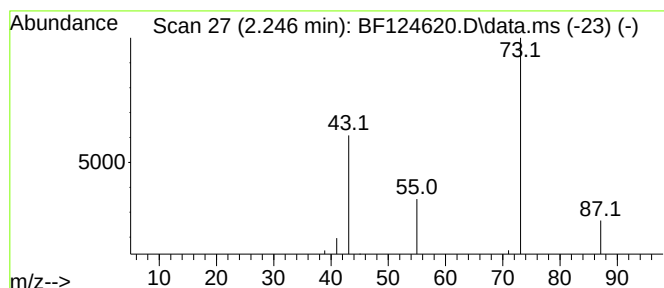
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.246	4.85 ng	8903	1,4-Dichlorobenzene-d4	6.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2			Isobutylamine	73	C4H11N	000078-81-9	5
3			1-Pentanamine	87	C5H13N	000110-58-7	4
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	4
5			3,4-Hexanediol, 2,5-dimethyl-	146	C8H18O2	022607-11-0	4



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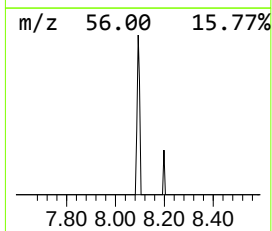
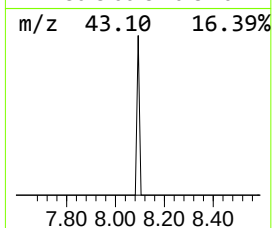
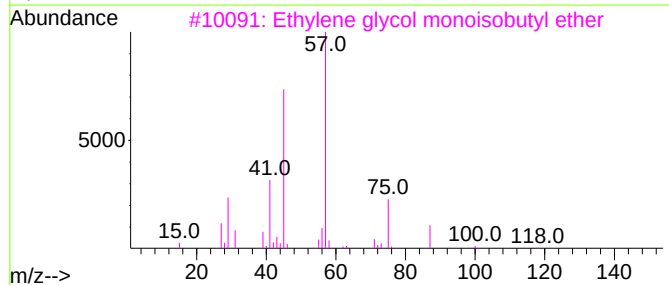
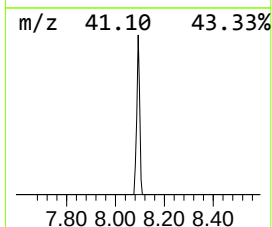
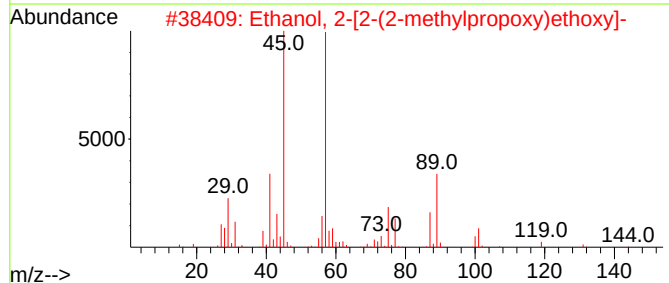
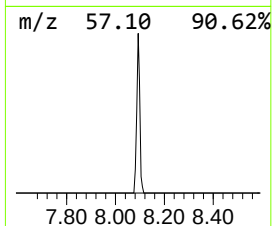
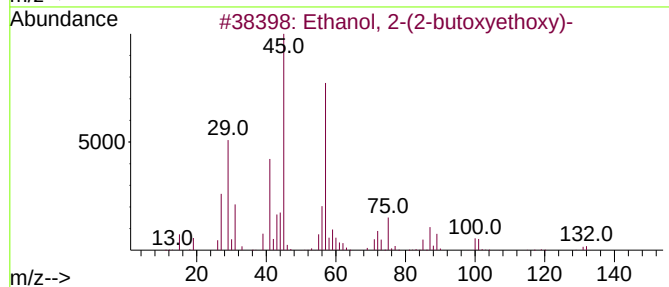
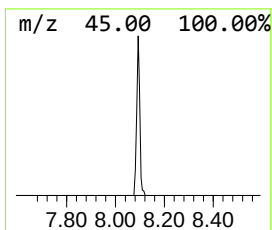
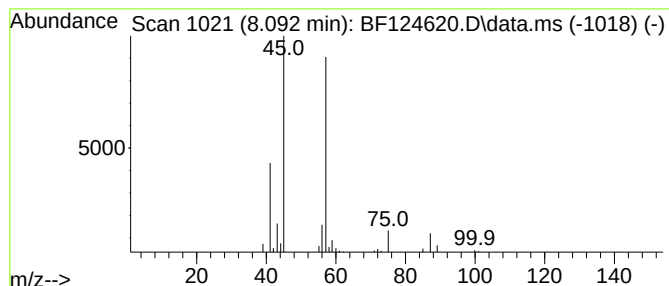
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	12.89 ng	33478	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	42
5			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	42



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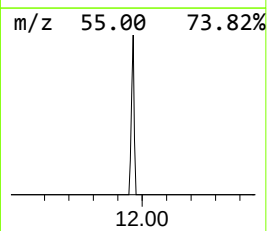
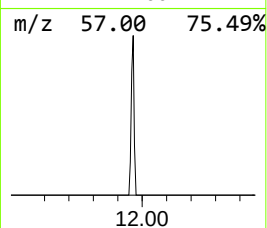
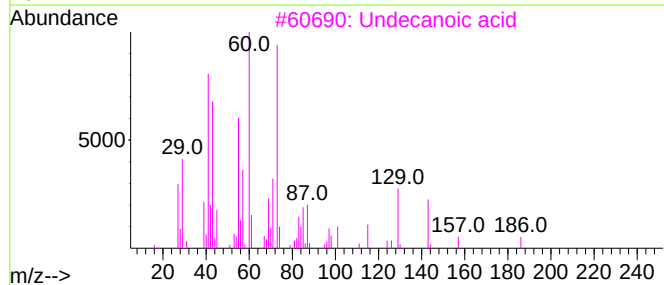
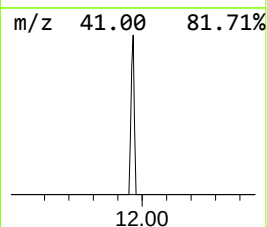
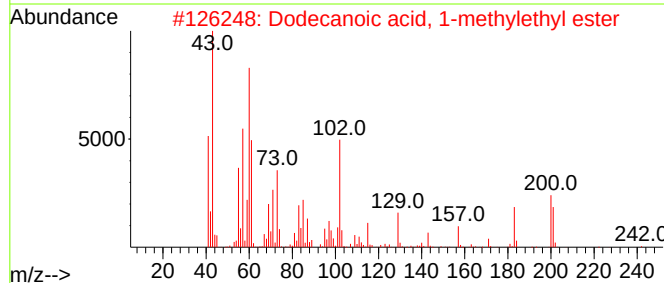
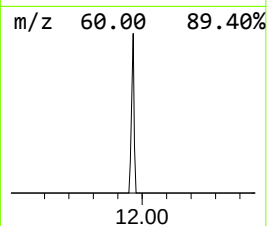
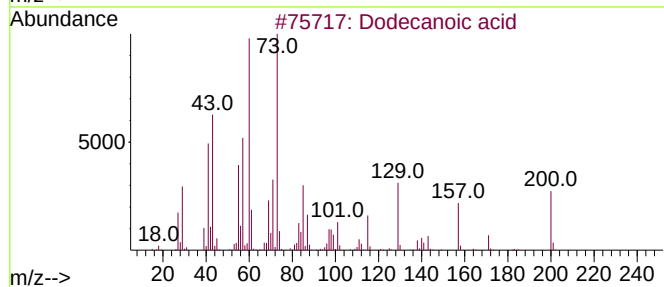
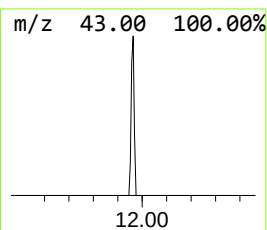
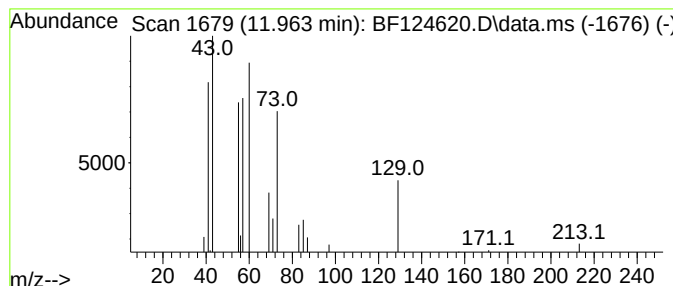
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Peak Number 3 Dodecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.963	3.37 ng	11246	Phenanthrene-d10	11.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	53
2			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	50
3			Undecanoic acid	186	C11H22O2	000112-37-8	40
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	37
5			Quinic acid	192	C7H12O6	000077-95-2	36



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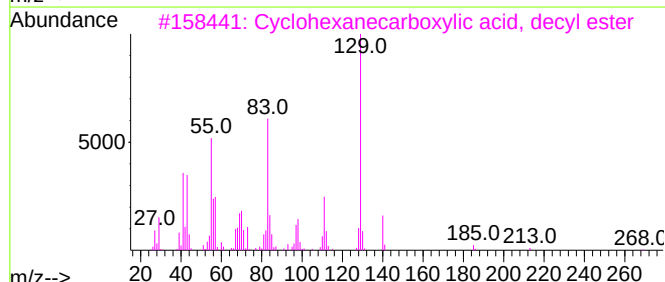
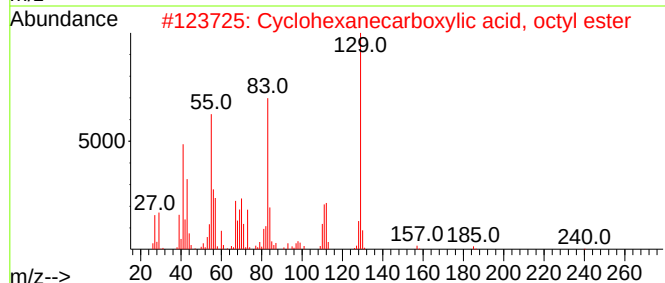
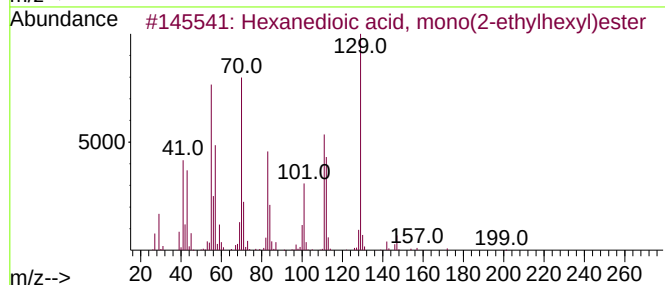
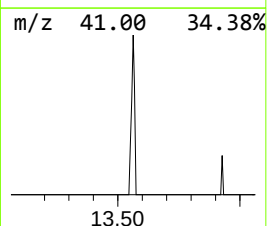
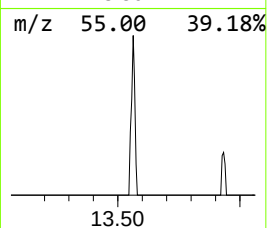
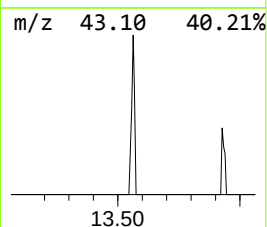
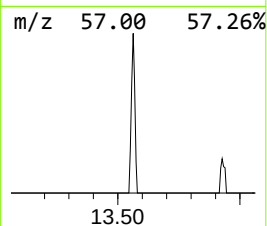
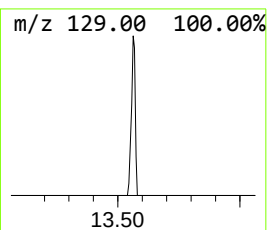
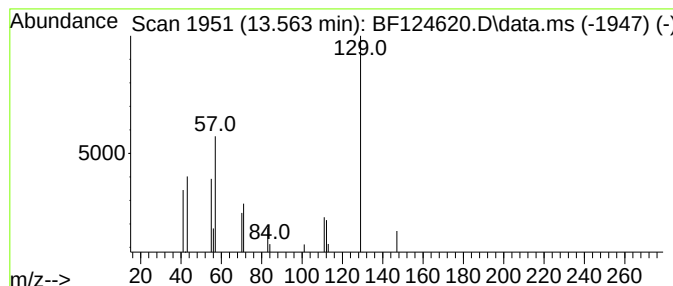
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Peak Number 4 Hexanedioic acid, mono(2-et... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.563	8.15 ng	17881	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	56
2			Cyclohexanecarboxylic acid, octy...	240	C15H28O2	089611-20-1	38
3			Cyclohexanecarboxylic acid, decy...	268	C17H32O2	093479-48-2	33
4			Thiophene, 2-nitro-	129	C4H3NO2S	000609-40-5	32
5			Succinic acid, ethyl 6-methylhep...	258	C14H26O4	1000381-35-9	28



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.246	4.8	ng	8903	1	6.910	36725	20.0
Ethanol, 2-(2-b...	8.092	12.9	ng	33478	2	8.198	51926	20.0
Dodecanoic acid	11.963	3.4	ng	11246	4	11.445	66788	20.0
Hexanedioic aci...	13.563	8.2	ng	17881	5	14.080	43895	20.0