

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072321\
 Data File : BF124708.D
 Acq On : 23 Jul 2021 11:29
 Operator : JU/CG
 Sample : M3129-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RO-VNJ-207

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-BF072221.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124708.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	10	14	18	rBB	15126	18760	7.75%	1.352%
2	5.104	510	513	517	rBB	2756	3649	1.51%	0.263%
3	5.487	573	578	581	rBB	190501	189267	78.15%	13.644%
4	6.493	743	749	752	rBB	161275	195544	80.74%	14.097%
5	6.869	810	813	816	rBB	54789	39021	16.11%	2.813%
6	7.434	904	909	912	rBB	134123	126080	52.06%	9.089%
7	8.051	1011	1014	1017	rBV	40471	27414	11.32%	1.976%
8	8.151	1027	1031	1034	rBB	70047	52549	21.70%	3.788%
9	9.228	1209	1214	1217	rBB	265642	242183	100.00%	17.459%
10	9.904	1326	1329	1332	rBB	70753	56625	23.38%	4.082%
11	10.698	1460	1464	1467	rBB	144612	125261	51.72%	9.030%
12	11.392	1579	1582	1585	rBB	66036	48714	20.11%	3.512%
13	11.916	1667	1671	1673	rBB	9928	8346	3.45%	0.602%
14	12.698	1802	1804	1806	rBB	5259	3859	1.59%	0.278%
15	12.980	1848	1852	1855	rBB	208722	177100	73.13%	12.767%
16	13.516	1937	1943	1944	rBV4	3541	4734	1.95%	0.341%
17	13.874	2000	2004	2007	rBV	7704	9990	4.12%	0.720%
18	14.027	2027	2030	2033	rBV	37303	30614	12.64%	2.207%
19	15.498	2276	2280	2284	rBV	25020	27440	11.33%	1.978%

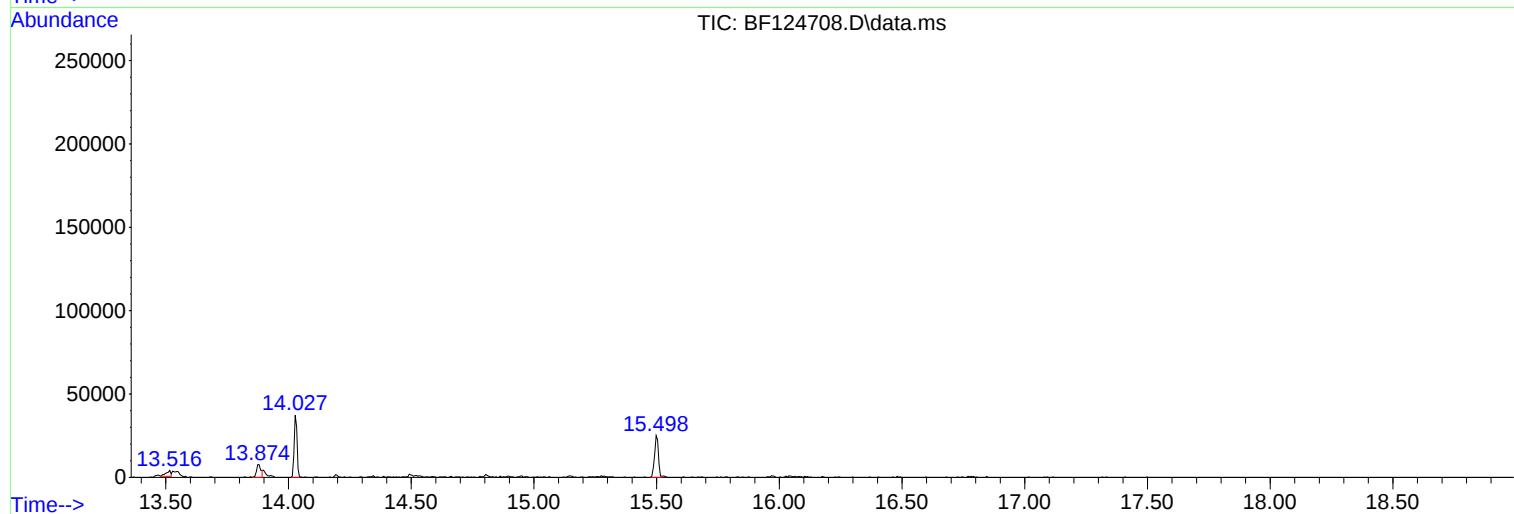
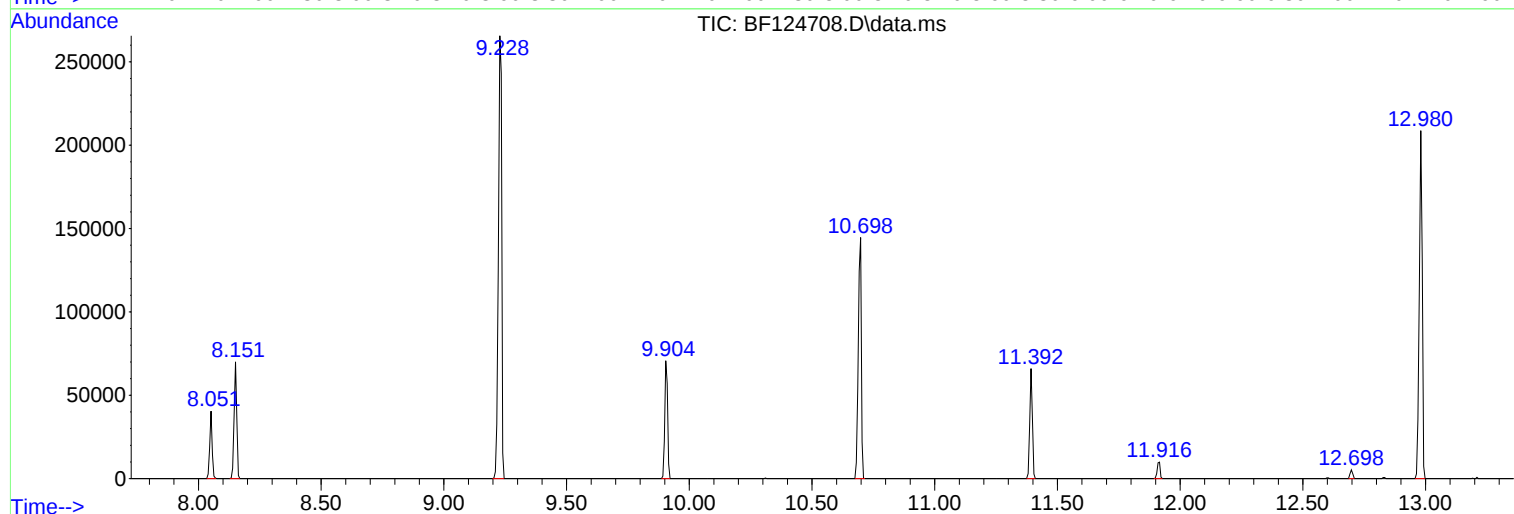
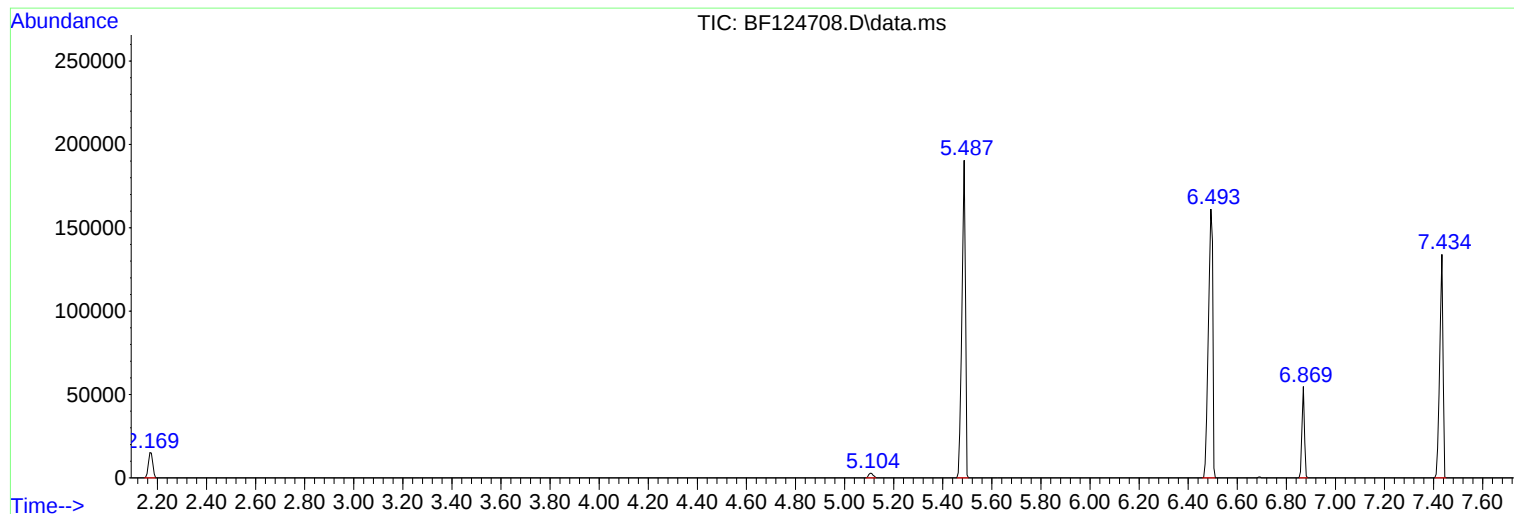
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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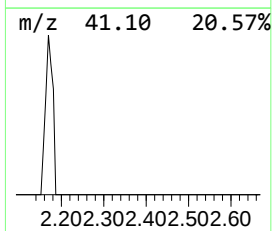
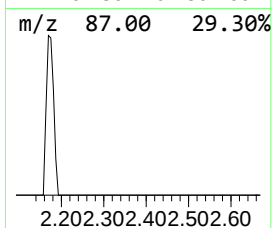
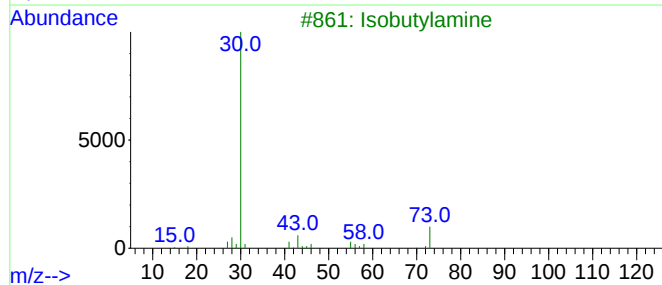
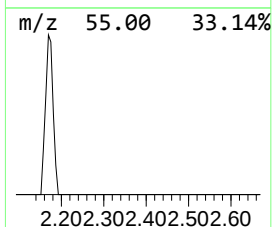
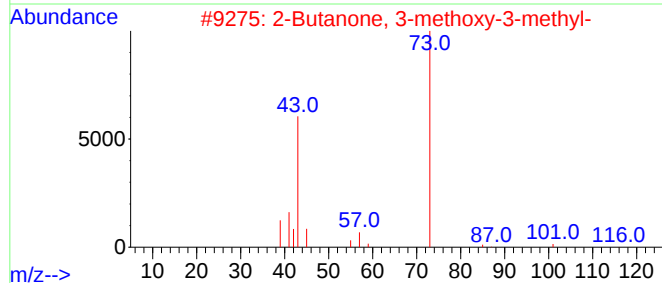
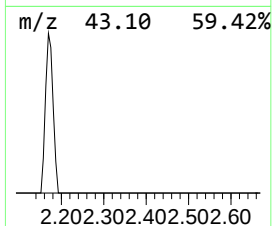
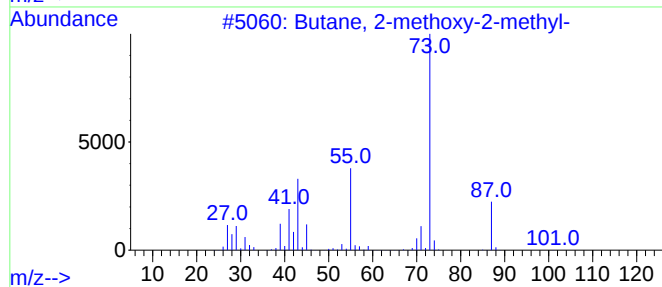
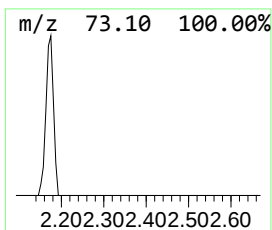
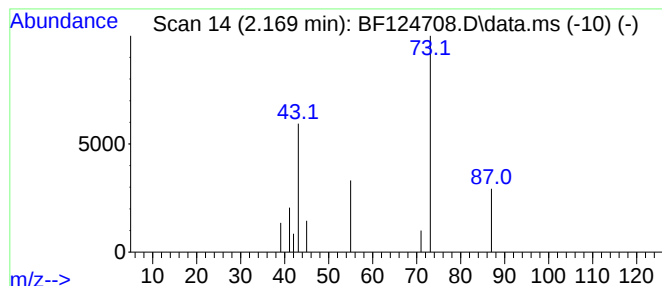
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	9.62 ng	18760	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2			2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9
3			Isobutylamine	73	C4H11N	000078-81-9	5
4			1-Pentanamine	87	C5H13N	000110-58-7	4
5			1,4-Butanediamine	88	C4H12N2	000110-60-1	4



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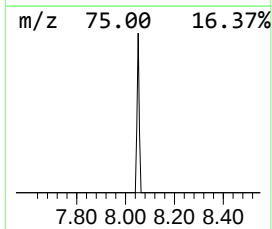
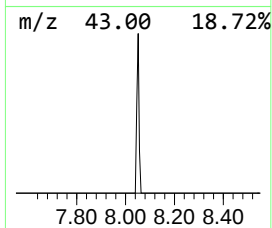
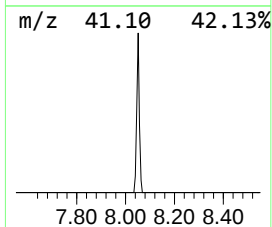
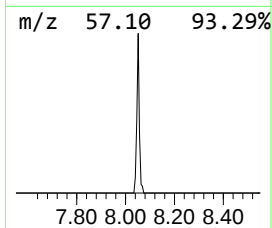
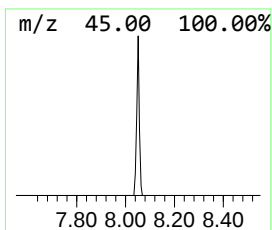
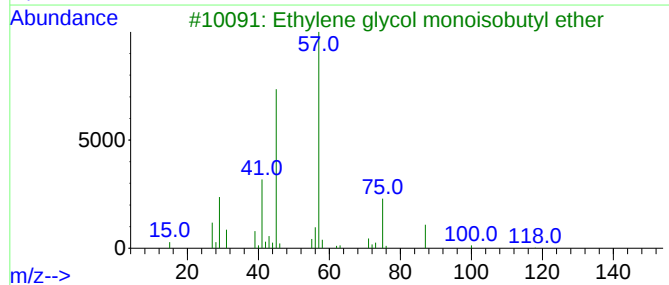
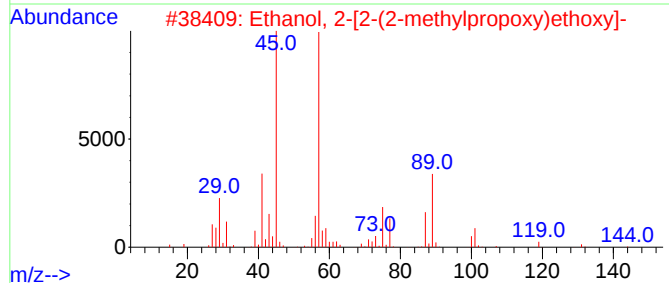
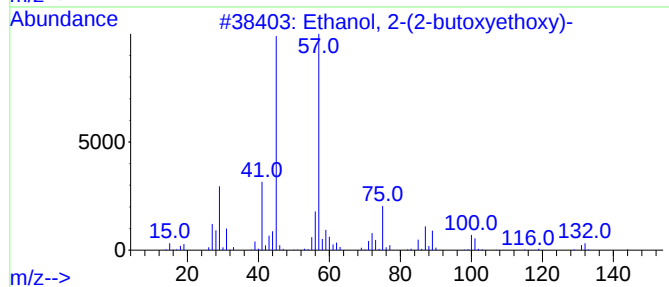
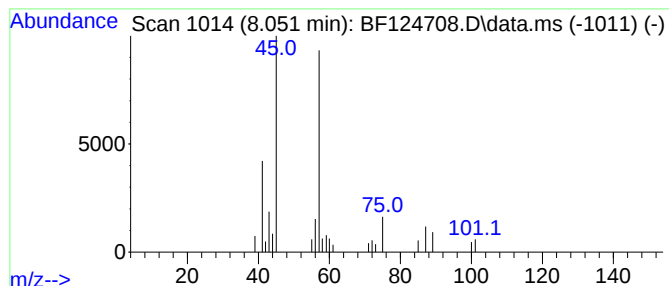
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	10.43 ng	27414	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	45
4			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	43
5			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	40



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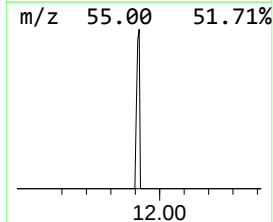
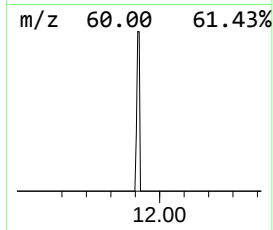
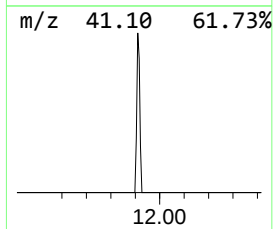
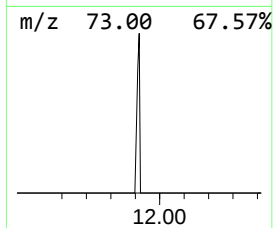
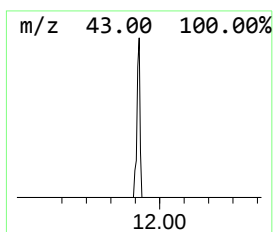
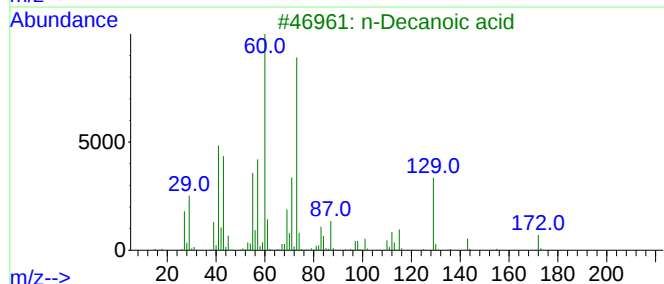
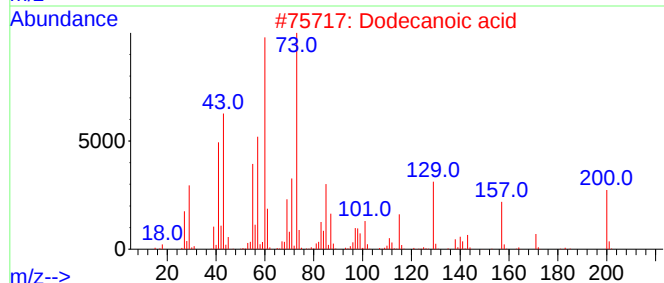
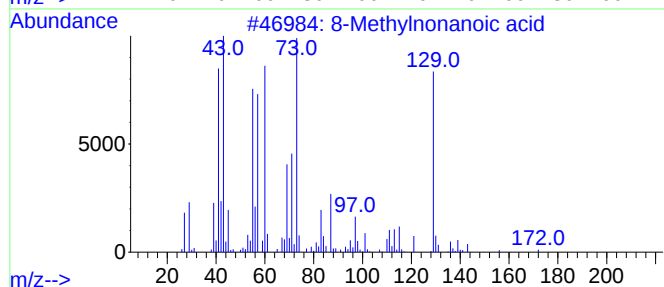
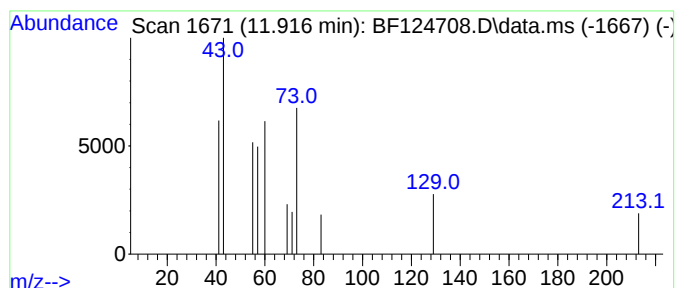
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown11.916 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.916	3.43 ng	8346	Phenanthrene-d10	11.392	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	40
2	Dodecanoic acid	200	C12H24O2	000143-07-7	38
3	n-Decanoic acid	172	C10H20O2	000334-48-5	38
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	33
5	Undecanoic acid, 10-bromo-	264	C11H21BrO2	018294-93-4	25



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Instrument :
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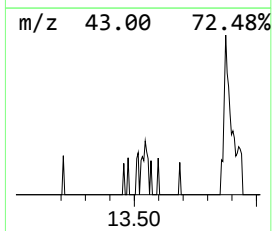
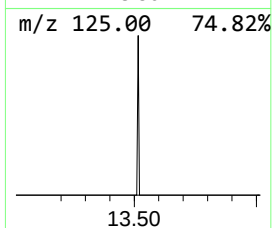
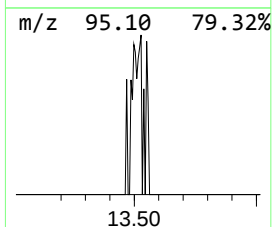
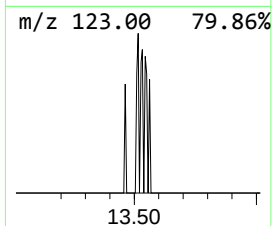
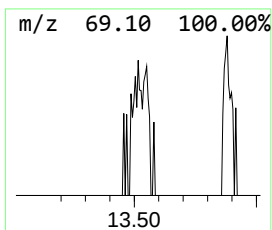
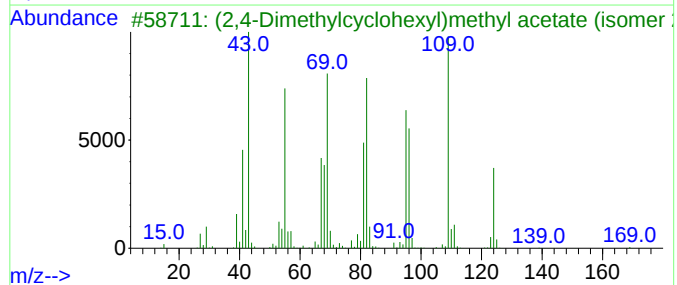
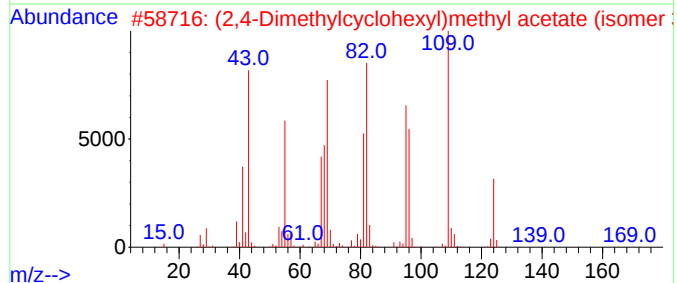
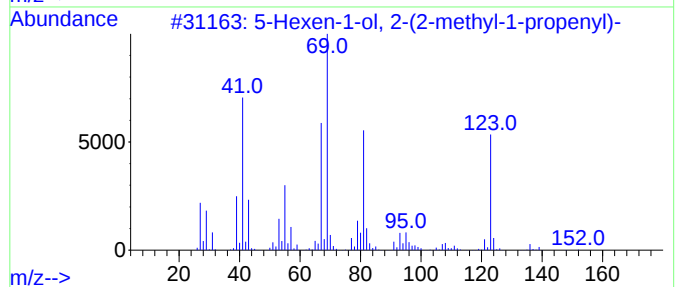
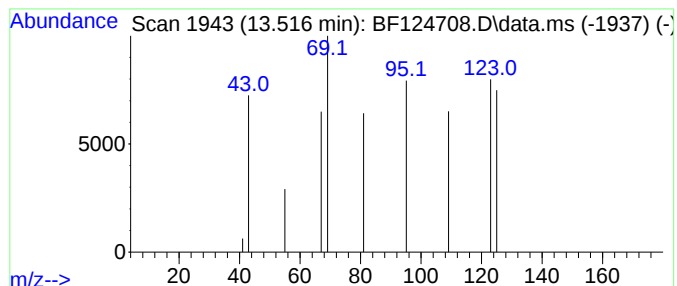
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown13.516 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.516	3.09 ng	4734	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Hexen-1-ol, 2-(2-methyl-1-prop...	154	C10H18O	018675-19-9	23		
2	(2,4-Dimethylcyclohexyl)methyl a...	184	C11H20O2	1000497-97-0	23		
3	(2,4-Dimethylcyclohexyl)methyl a...	184	C11H20O2	1000497-96-9	23		
4	2-Tridecyne	180	C13H24	028467-75-6	10		
5	1-Methyl-2-methylenecyclohexane	110	C8H14	002808-75-5	9		



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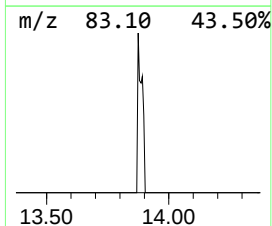
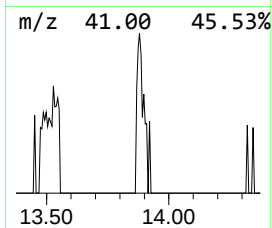
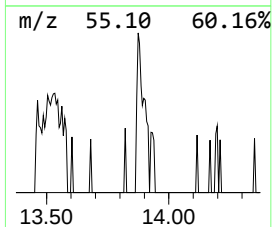
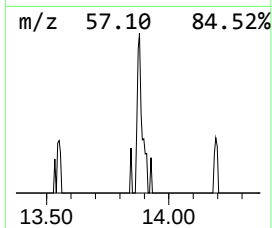
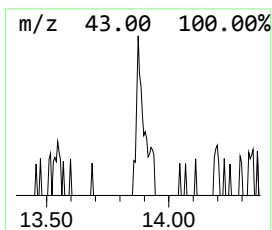
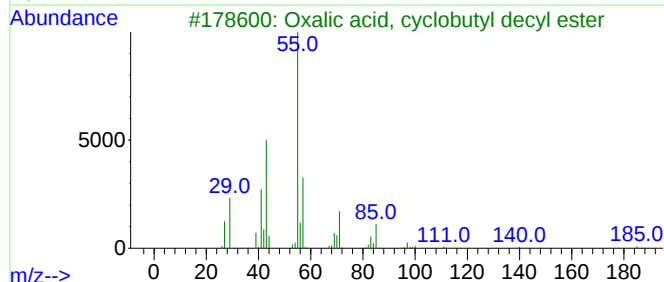
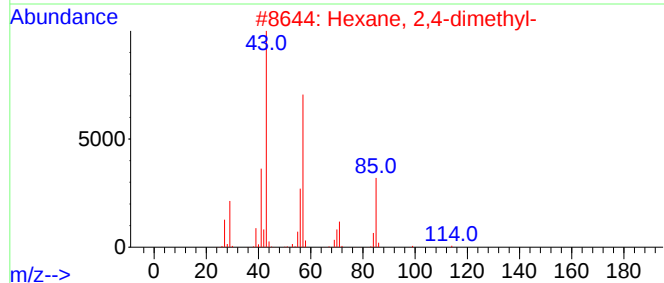
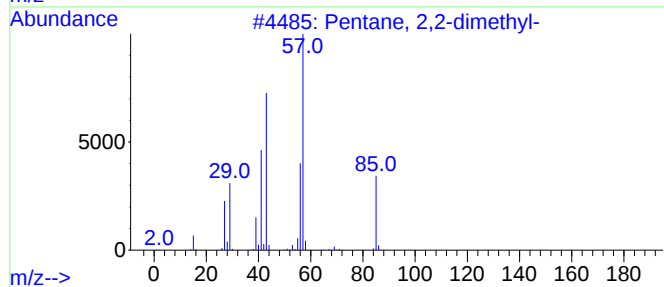
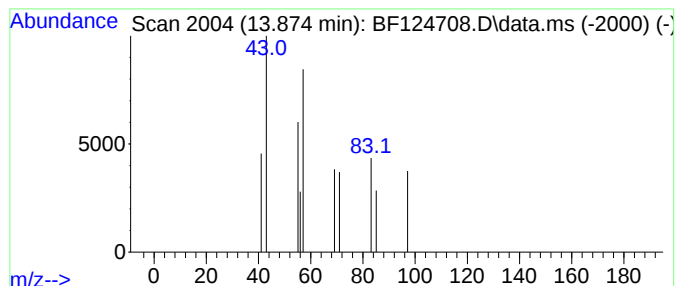
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown13.874 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	6.53 ng	9990	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	9
2			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	9
3			Oxalic acid, cyclobutyl decyl ester	284	C16H28O4	1000309-70-1	9
4			Oxalic acid, cyclobutyl nonyl ester	270	C15H26O4	1000309-70-0	9
5			Acetyl valeryl	128	C7H12O2	000096-04-8	9



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.169	9.6	ng	18760	1	6.869	39021	20.0
Ethanol, 2-(2-b...	8.051	10.4	ng	27414	2	8.151	52549	20.0
unknown11.916	11.916	3.4	ng	8346	4	11.392	48714	20.0
unknown13.516	13.516	3.1	ng	4734	5	14.027	30614	20.0
unknown13.874	13.874	6.5	ng	9990	5	14.027	30614	20.0