

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072321\
 Data File : BF124728.D
 Acq On : 23 Jul 2021 23:31
 Operator : JU/CG
 Sample : M3138-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VB16085

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: BF124728.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	16	21	24	rBB	15424	18590	7.02%	1.127%
2	5.116	512	515	520	rBB	3255	3773	1.42%	0.229%
3	5.493	574	579	582	rBB	211879	214898	81.16%	13.028%
4	6.498	743	750	752	rBB	191875	222246	83.93%	13.473%
5	6.869	810	813	816	rBB	48561	36246	13.69%	2.197%
6	7.434	904	909	911	rBB	142865	144463	54.56%	8.758%
7	8.051	1010	1014	1017	rBB	42211	31417	11.86%	1.905%
8	8.151	1027	1031	1034	rBB	61686	50825	19.19%	3.081%
9	9.228	1209	1214	1217	rBB	293464	264796	100.00%	16.053%
10	9.904	1325	1329	1332	rBB	76341	59601	22.51%	3.613%
11	10.698	1459	1464	1467	rBB	211169	182377	68.87%	11.056%
12	11.392	1578	1582	1585	rBB	77868	59742	22.56%	3.622%
13	11.916	1668	1671	1674	rBB	27162	19495	7.36%	1.182%
14	12.698	1802	1804	1807	rBB	11198	8236	3.11%	0.499%
15	12.980	1848	1852	1855	rBV	265891	257073	97.08%	15.585%
16	13.869	2000	2003	2006	rBV2	5324	5324	2.01%	0.323%
17	13.898	2006	2008	2010	rVB	4992	3659	1.38%	0.222%
18	14.027	2027	2030	2033	rBB	48294	38491	14.54%	2.333%
19	15.498	2276	2280	2284	rBB2	26359	28262	10.67%	1.713%

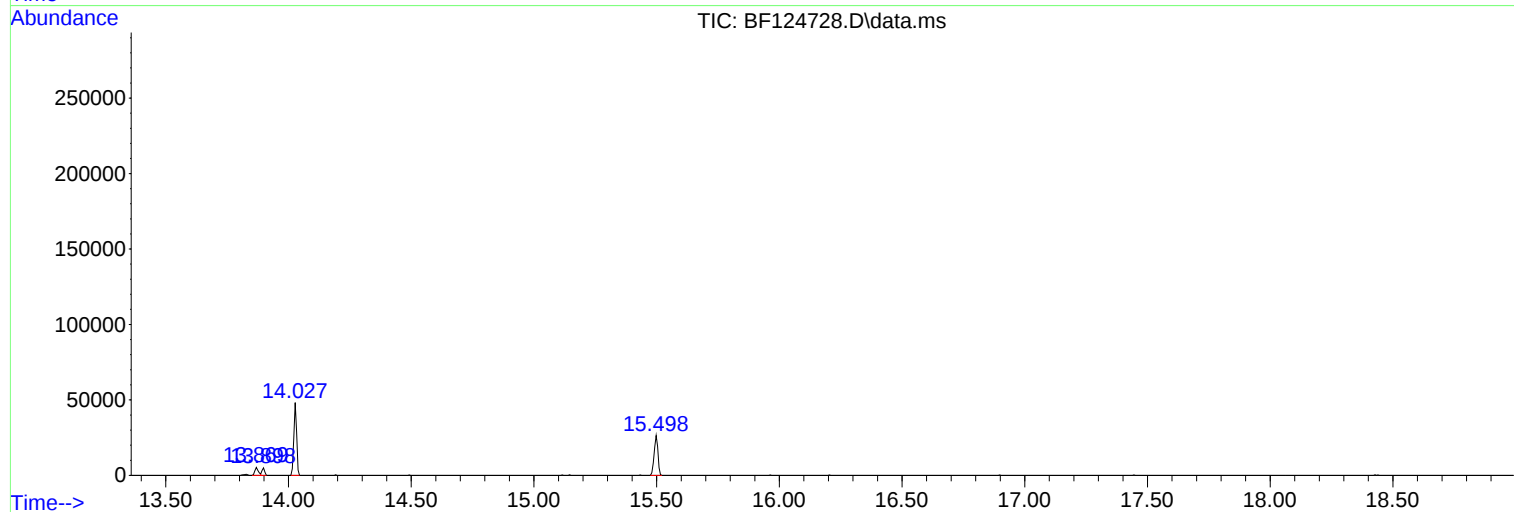
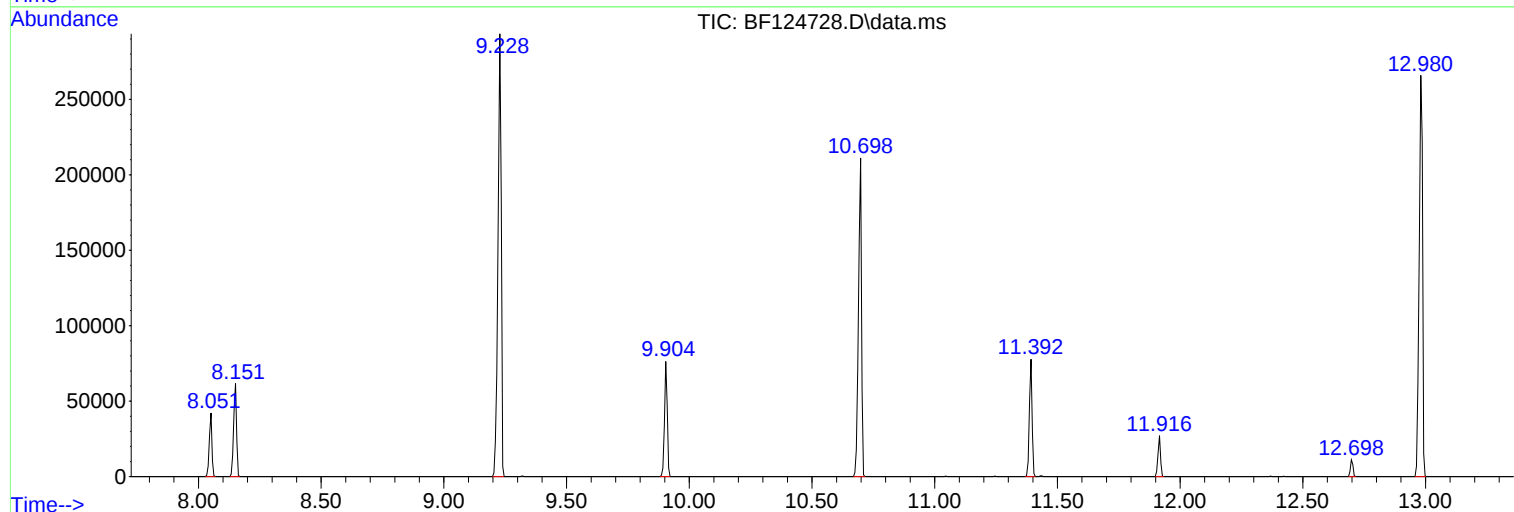
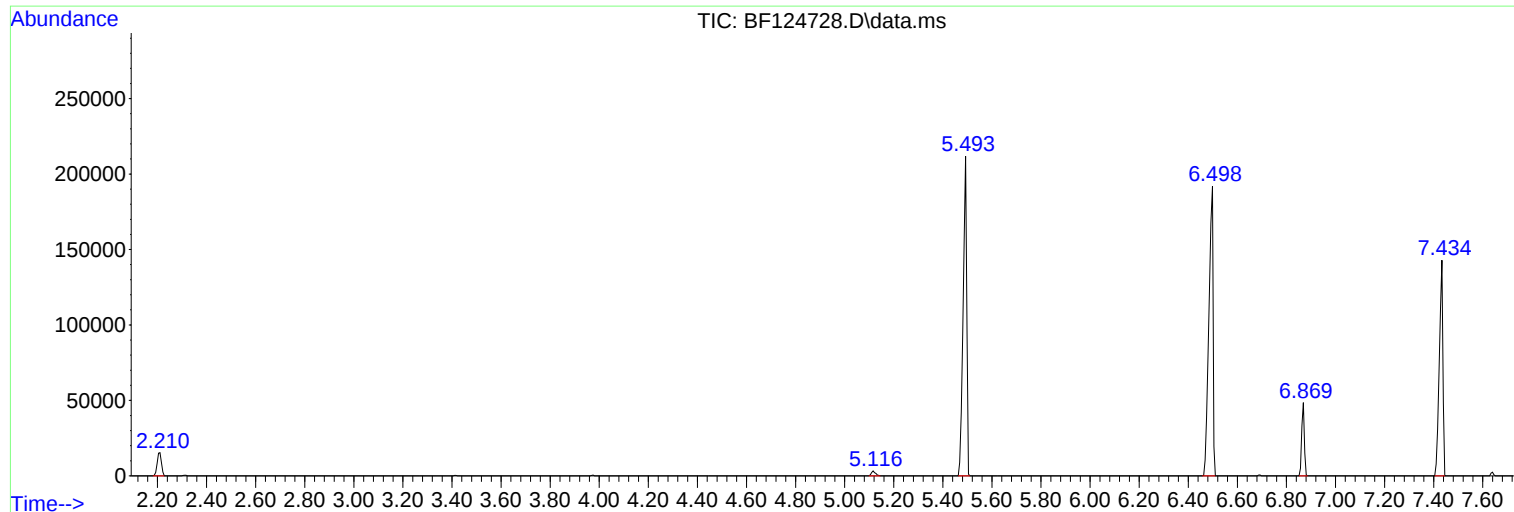
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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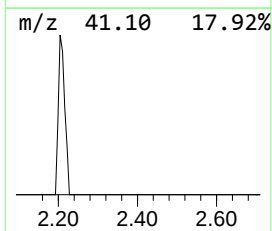
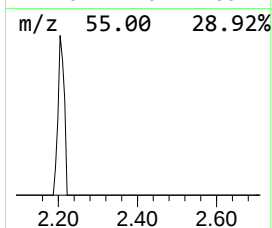
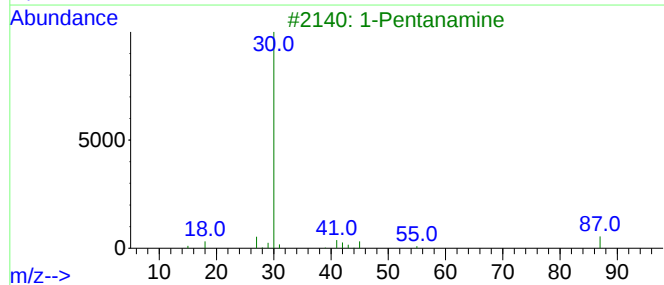
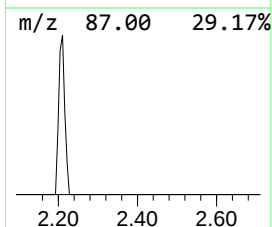
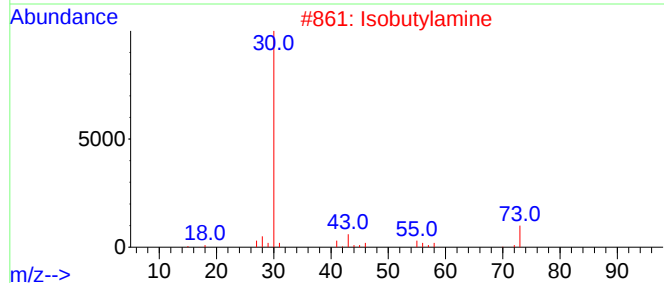
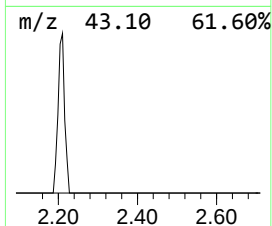
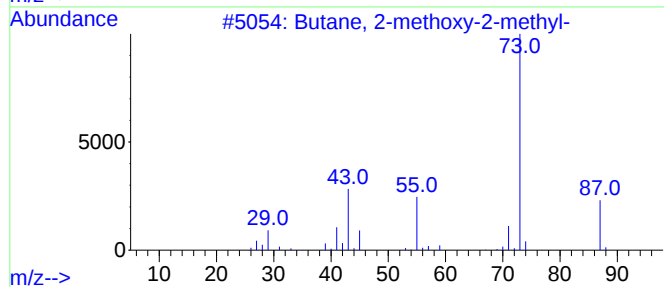
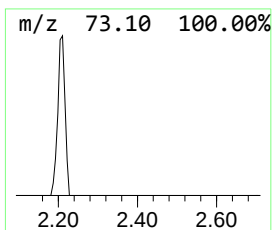
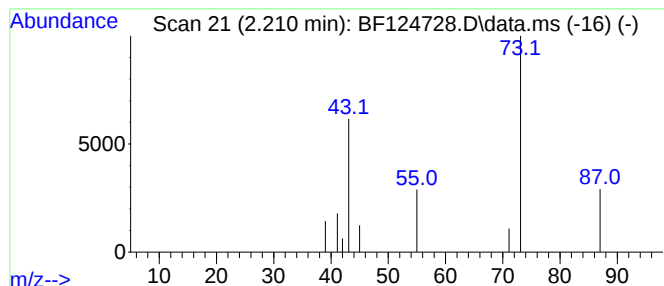
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.210	10.26 ng	18590	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	83
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		2-OXOPROPIONAMIDE	87	C3H5NO2	000631-66-3	4



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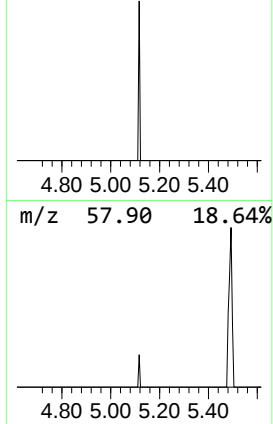
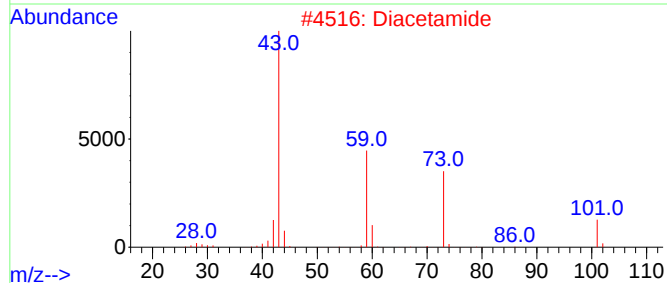
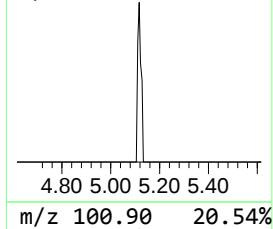
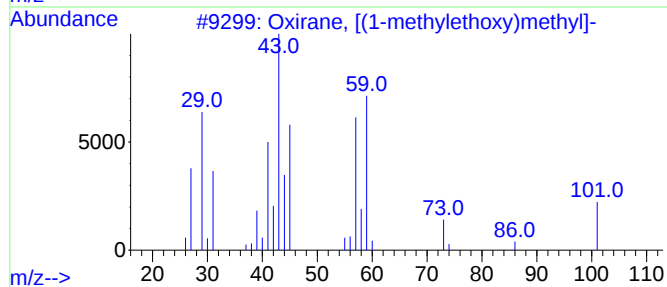
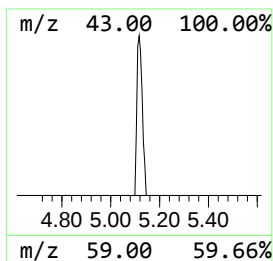
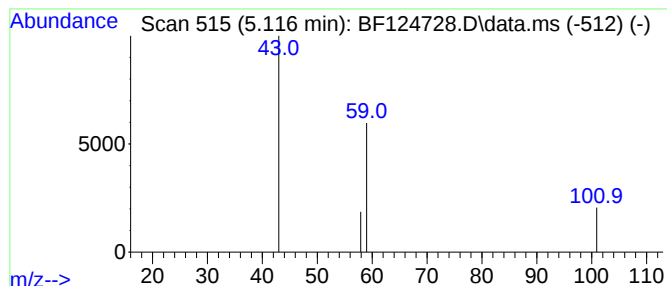
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown5.116 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	2.08 ng	3773	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	9
2			Diacetamide	101	C4H7NO2	000625-77-4	4
3			Guanidine	59	CH5N3	000113-00-8	4
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	4
5			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	4



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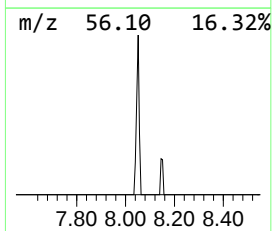
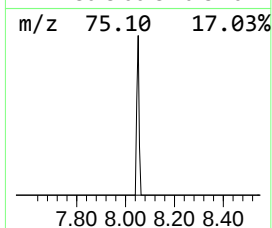
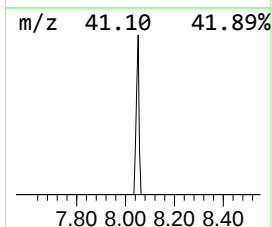
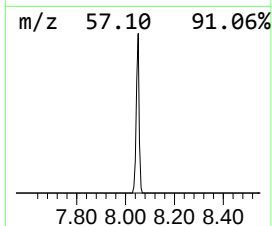
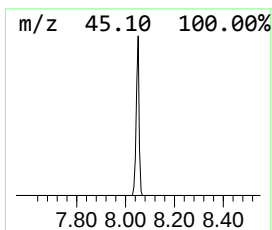
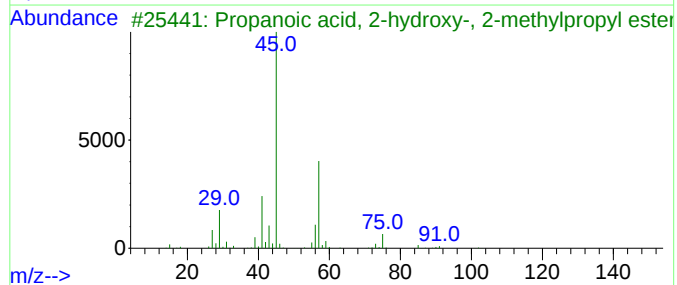
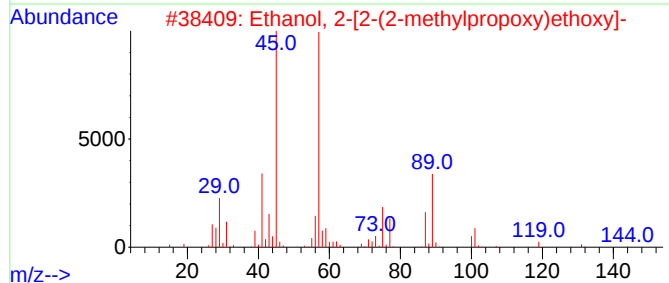
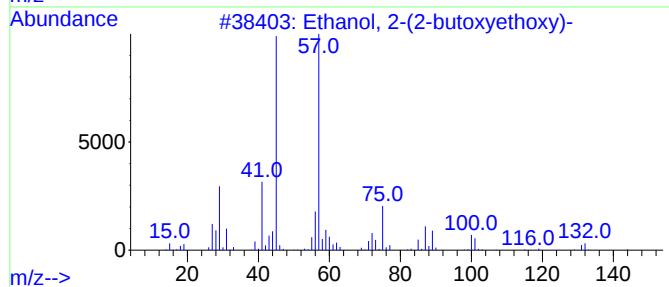
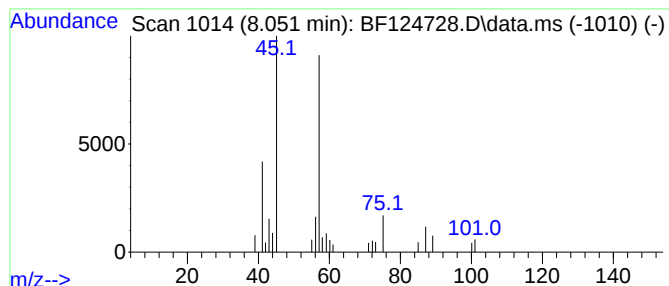
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	12.36 ng	31417	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			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	53
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
5			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	42



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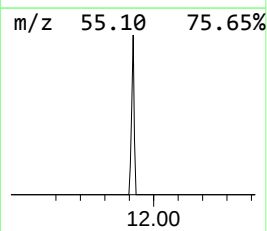
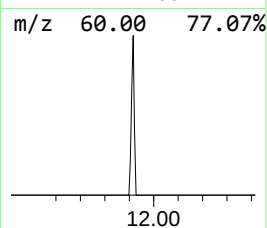
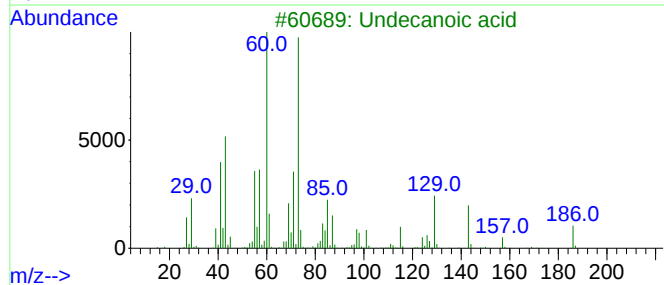
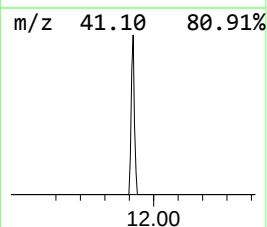
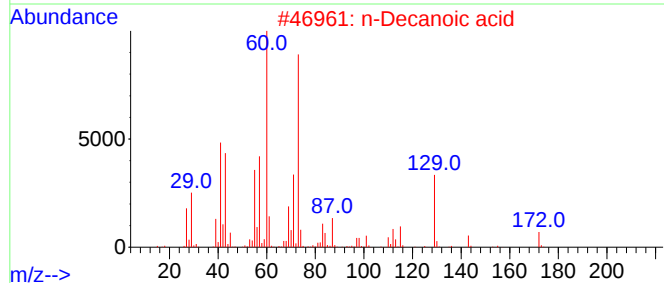
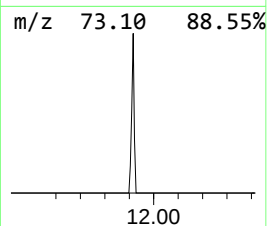
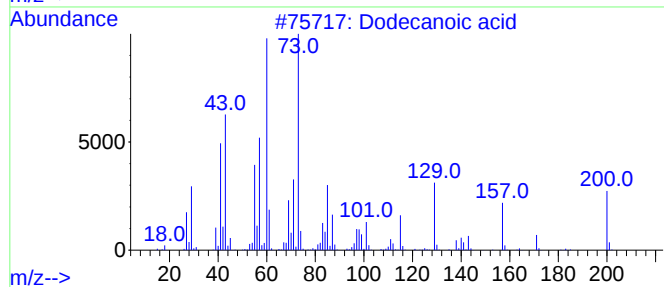
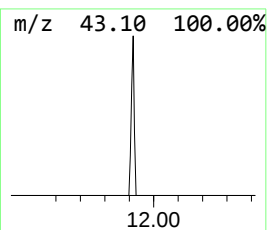
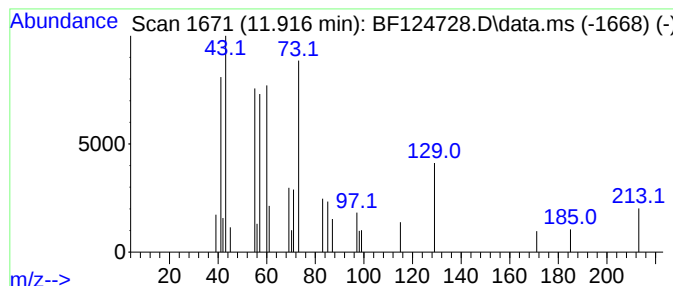
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Dodecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	6.53 ng	19495	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	59
2			n-Decanoic acid	172	C10H20O2	000334-48-5	50
3			Undecanoic acid	186	C11H22O2	000112-37-8	47
4			Octanoic acid	144	C8H16O2	000124-07-2	43
5			.beta.-D-Glucopyranoside, methyl...	292	C14H28O6	1010157-04-9	43



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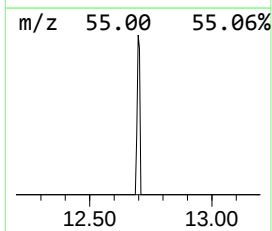
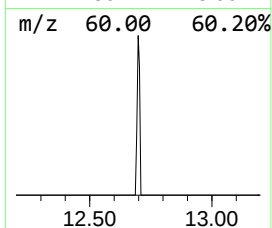
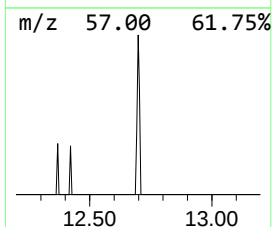
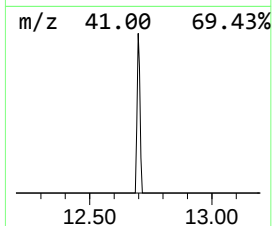
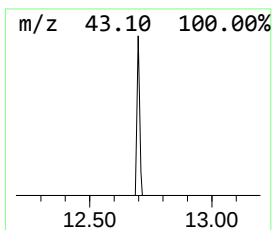
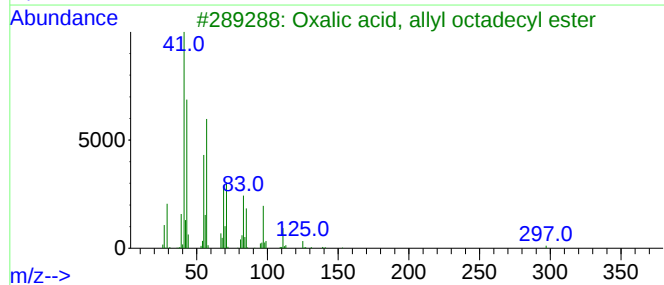
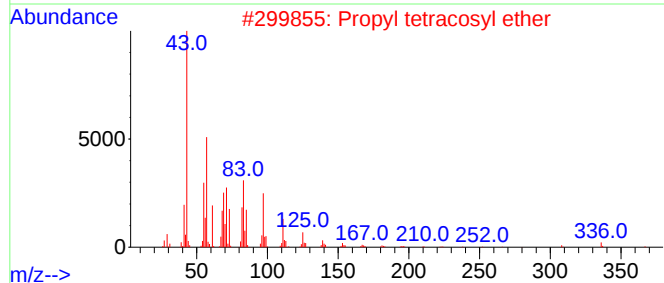
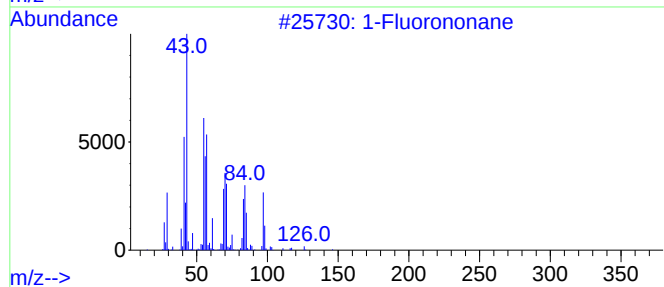
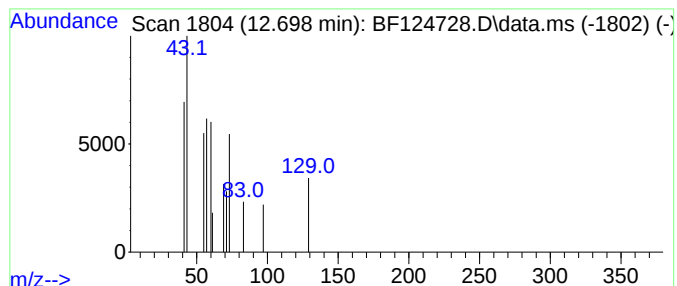
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown12.698 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.698	2.76 ng	8236	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Fluorononane	146	C9H19F	000463-18-3	38
2			Propyl tetracosyl ether	396	C27H56O	1000406-28-3	38
3			Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	35
4			Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	17
5			N-(3-Methylbutyl)acetamide	129	C7H15NO	013434-12-3	9



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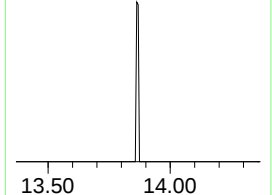
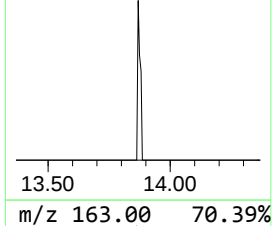
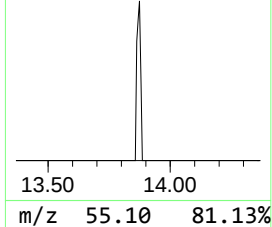
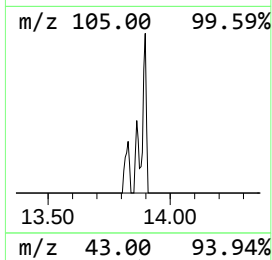
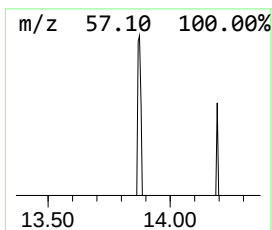
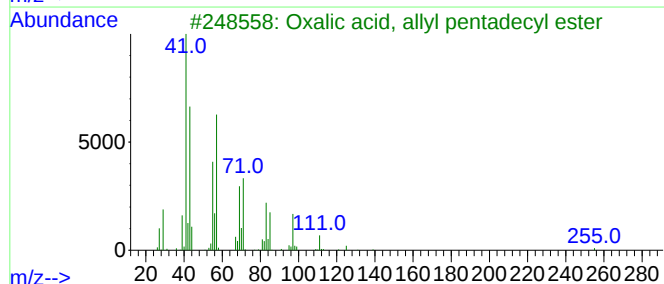
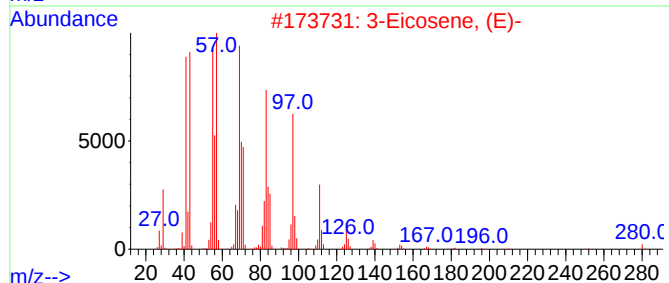
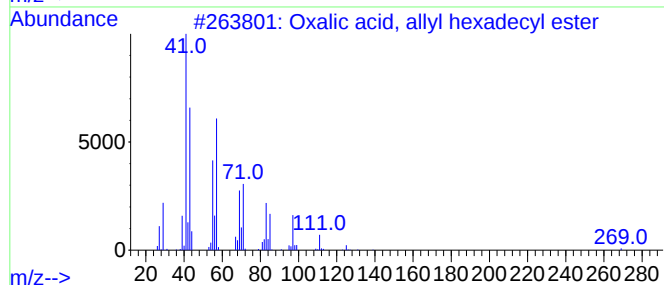
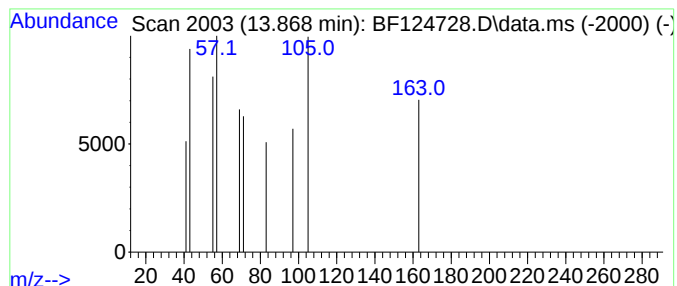
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown13.868 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	2.77 ng	5324	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	47
2			3-Eicosene, (E)-	280	C20H40	074685-33-9	47
3			Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	47
4			Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	42
5			Dotriacontyl propyl ether	509	C35H72O	1000406-28-7	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072321\
Data File : BF124728.D
Acq On : 23 Jul 2021 23:31
Operator : JU/CG
Sample : M3138-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VB16085

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.210	10.3	ng	18590	1	6.869	36246	20.0
unknown5.116	5.116	2.1	ng	3773	1	6.869	36246	20.0
Ethanol, 2-(2-b...	8.051	12.4	ng	31417	2	8.151	50825	20.0
Dodecanoic acid	11.916	6.5	ng	19495	4	11.392	59742	20.0
unknown12.698	12.698	2.8	ng	8236	4	11.392	59742	20.0
unknown13.868	13.868	2.8	ng	5324	5	14.027	38491	20.0