

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
 Data File : BF124643.D
 Acq On : 20 Jul 2021 23:46
 Operator : JU/CG
 Sample : M3043-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-077

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: BF124643.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	19	22	25	rBB	7655	7755	4.14%	0.690%
2	5.134	515	518	521	rBB2	2494	2948	1.57%	0.262%
3	5.516	578	583	586	rBB	157473	153729	81.99%	13.687%
4	6.522	748	754	757	rBB	150420	162056	86.43%	14.428%
5	6.904	815	819	821	rBB	44451	38071	20.30%	3.389%
6	7.463	909	914	917	rBB	109402	106270	56.68%	9.461%
7	8.081	1016	1019	1022	rBB	22471	15791	8.42%	1.406%
8	8.186	1033	1037	1040	rBB	69128	53750	28.67%	4.785%
9	9.263	1215	1220	1223	rBB	239613	187502	100.00%	16.693%
10	9.939	1332	1335	1338	rBB	68659	58647	31.28%	5.221%
11	10.727	1466	1469	1472	rBB	122242	109237	58.26%	9.725%
12	11.427	1585	1588	1591	rBB	62167	47562	25.37%	4.234%
13	11.945	1674	1676	1679	rBB	13822	10735	5.73%	0.956%
14	12.733	1808	1810	1812	rBB	3580	2693	1.44%	0.240%
15	13.015	1854	1858	1861	rBB	132705	104355	55.66%	9.291%
16	13.910	2008	2010	2016	rBB2	8815	8350	4.45%	0.743%
17	14.068	2034	2037	2040	rBB	28709	23546	12.56%	2.096%
18	14.533	2113	2116	2121	rBB	3285	3823	2.04%	0.340%
19	15.192	2225	2228	2232	rBB	3409	3372	1.80%	0.300%
20	15.557	2285	2290	2293	rBV	19985	23018	12.28%	2.049%

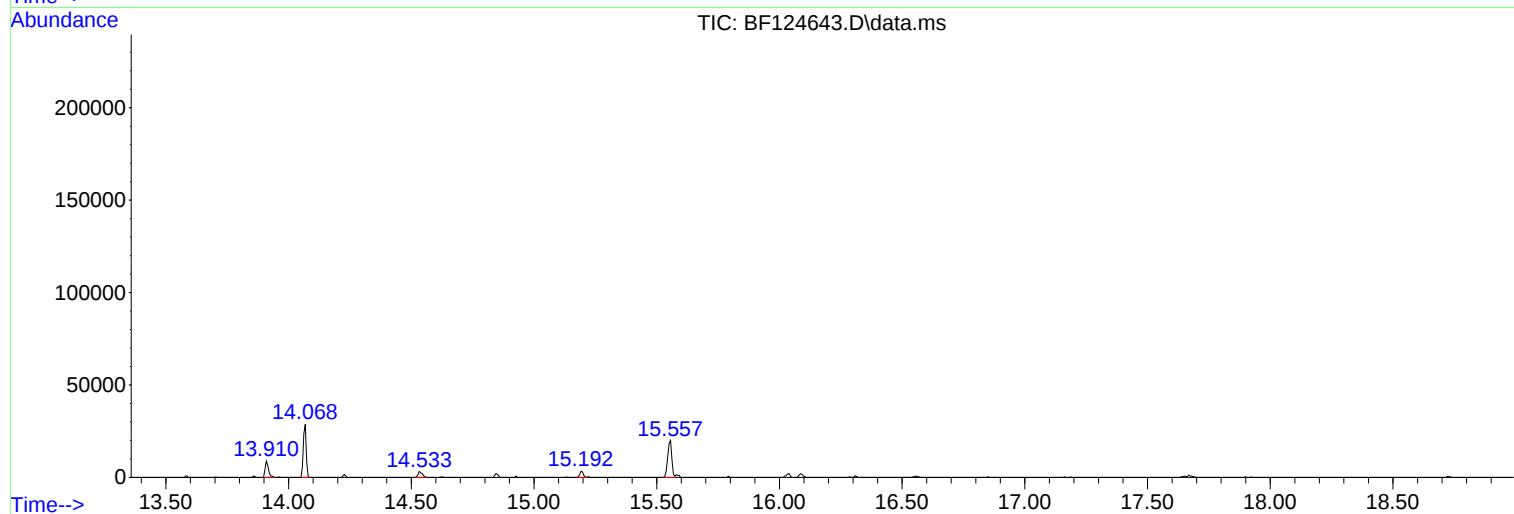
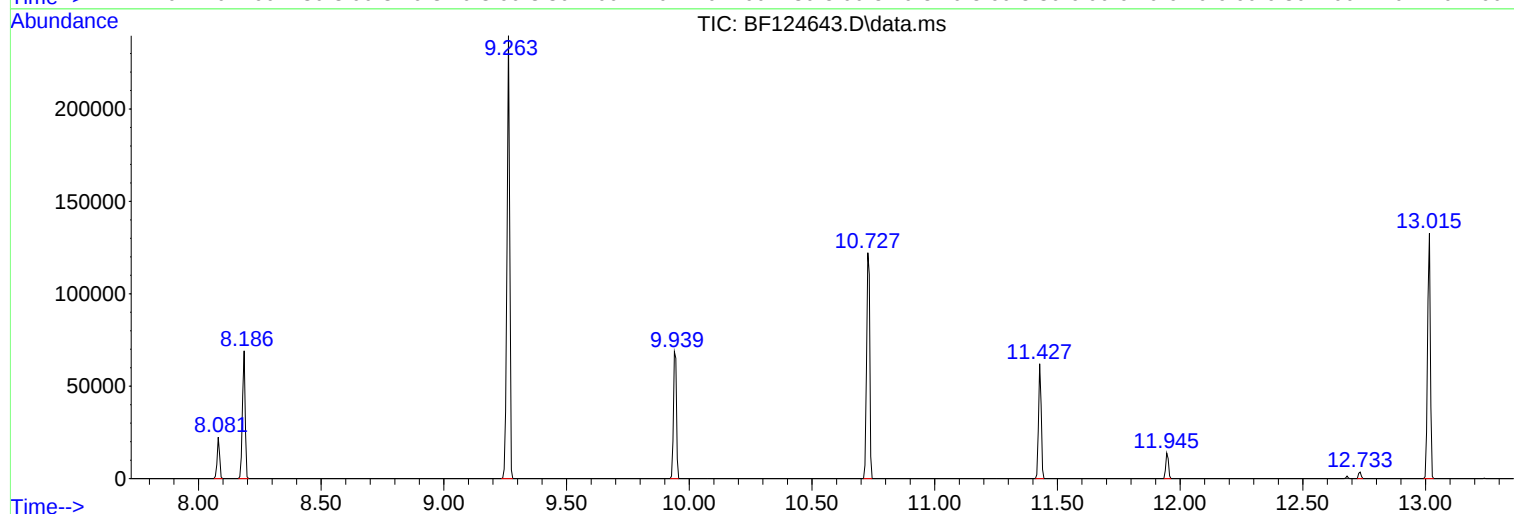
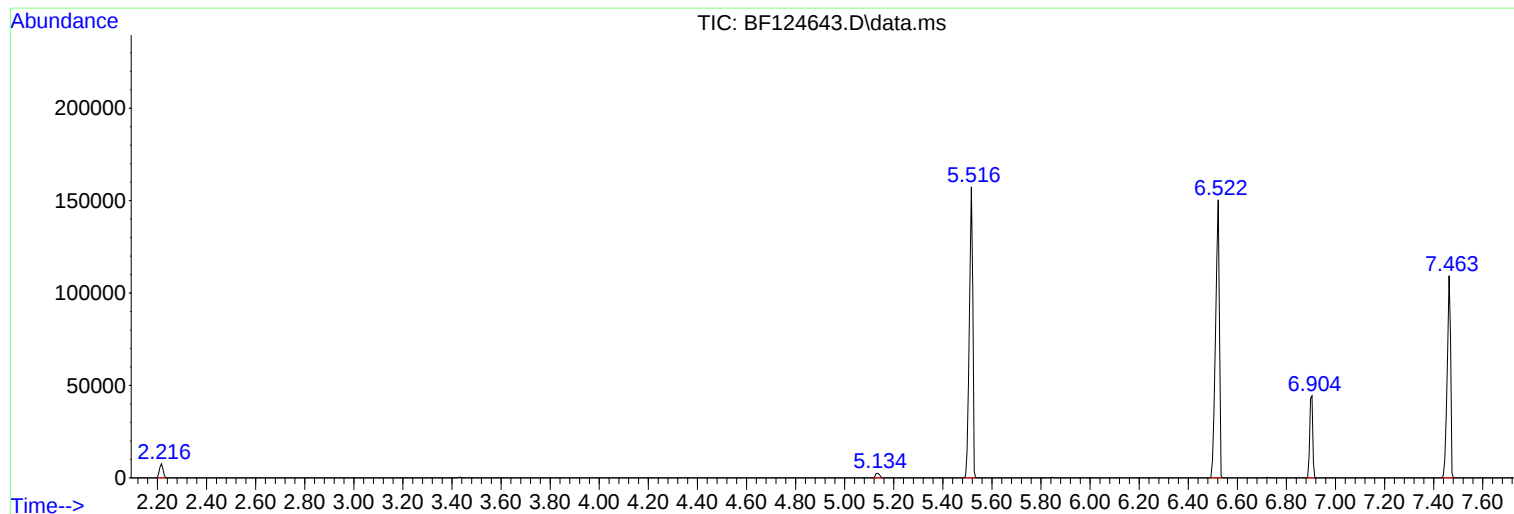
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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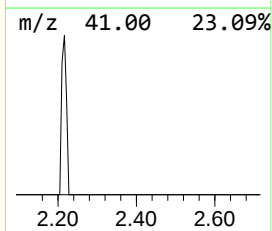
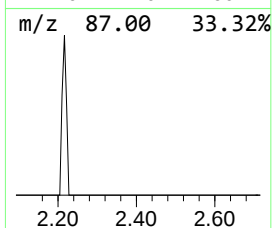
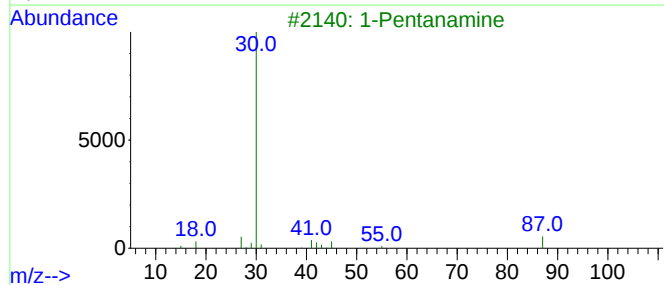
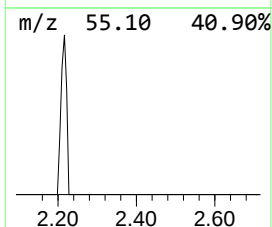
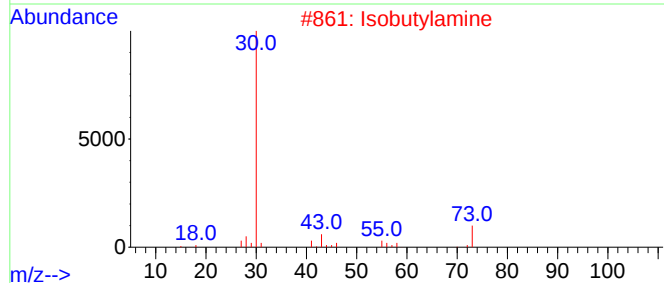
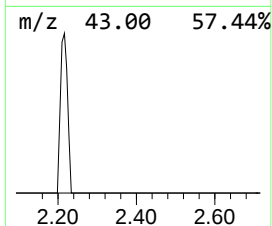
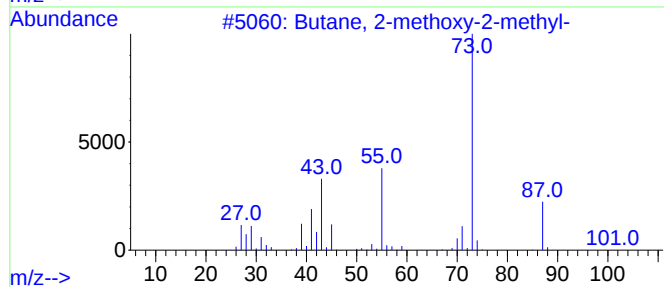
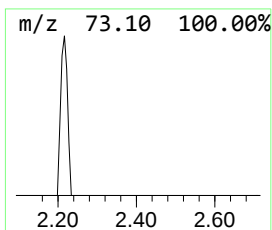
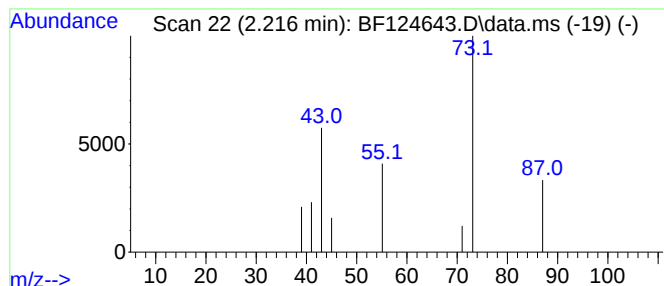
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	4.07 ng	7755	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			Isobutylamine	73	C4H11N	000078-81-9	5
3			1-Pentanamine	87	C5H13N	000110-58-7	4
4			2-OXOPROPIONAMIDE	87	C3H5NO2	000631-66-3	4
5			3,4-Hexanediol, 2,5-dimethyl-	146	C8H18O2	022607-11-0	4



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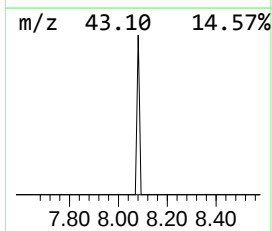
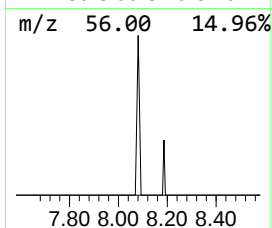
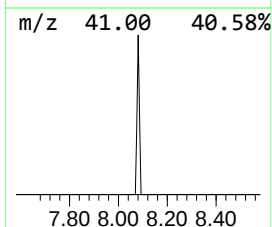
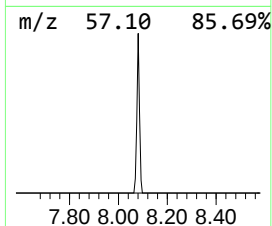
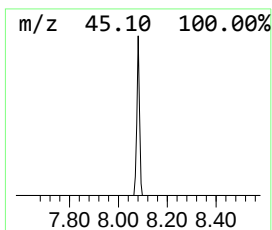
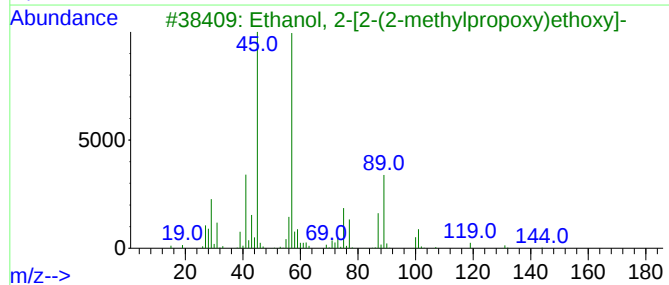
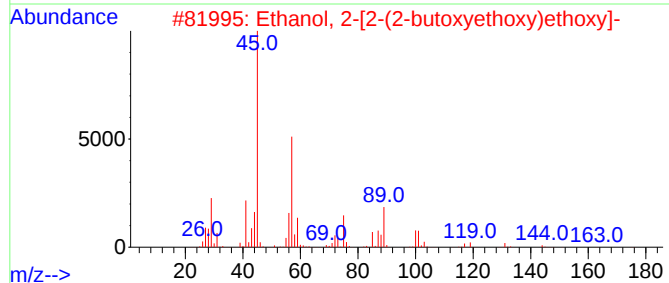
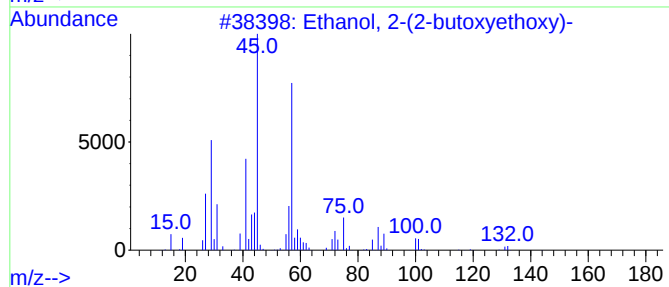
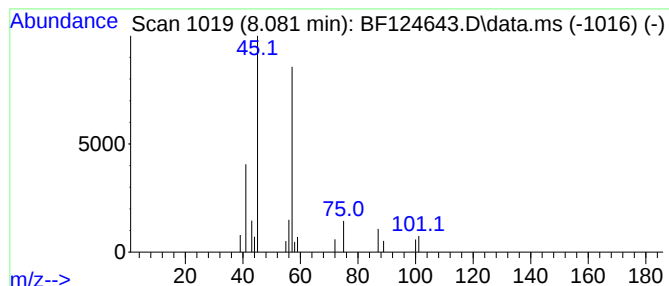
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.081	5.88 ng	15791	Naphthalene-d8	8.186

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	56
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	38
5			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	36



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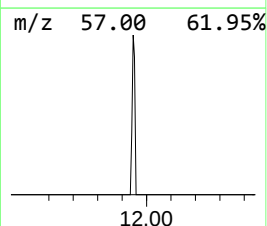
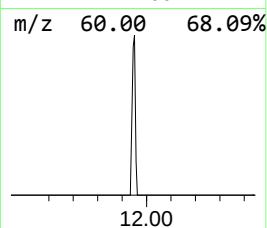
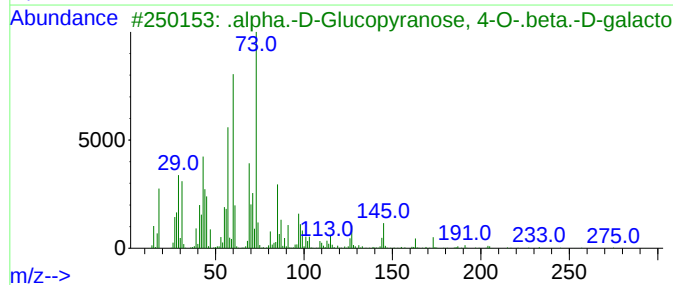
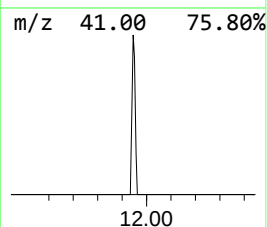
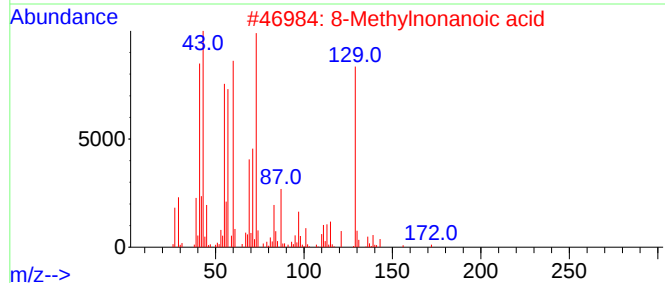
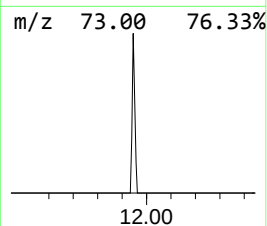
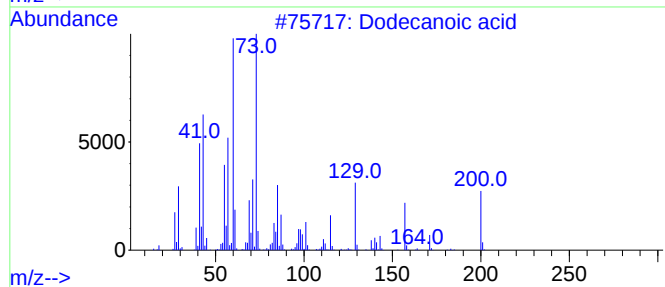
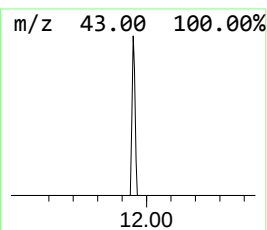
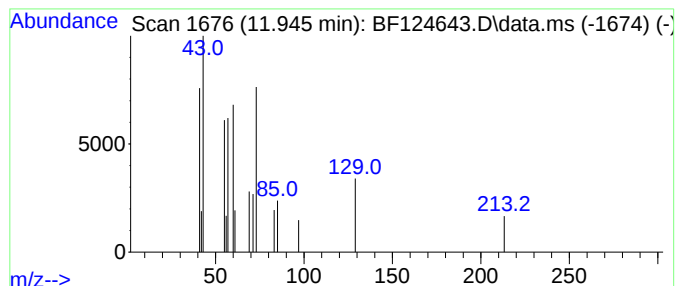
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Peak Number 3 Dodecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	4.51 ng	10735	Phenanthrene-d10	11.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	59
2			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	40
3			.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	40
4			1-(p-Toluidino)-1-deoxy-.beta.-d...	269	C13H19NO5	1000226-06-4	37
5			Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	35



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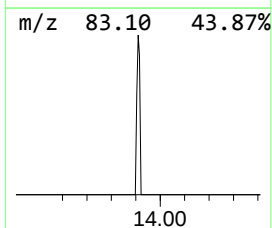
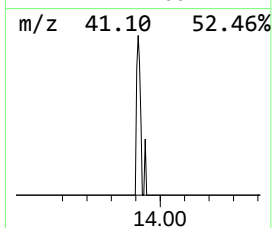
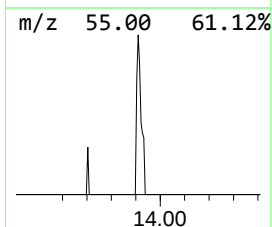
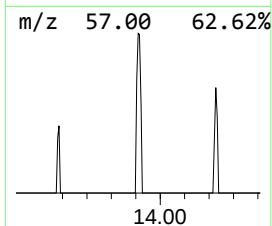
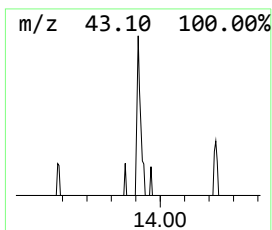
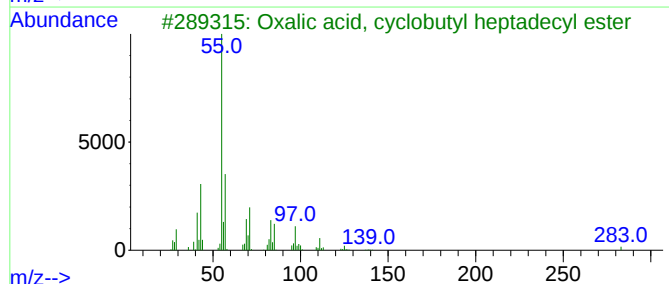
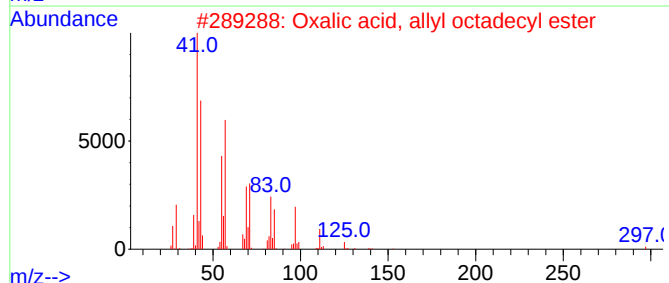
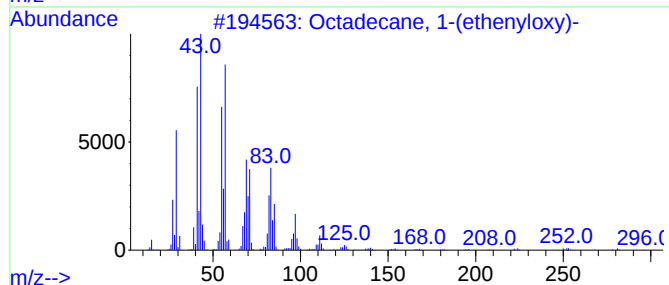
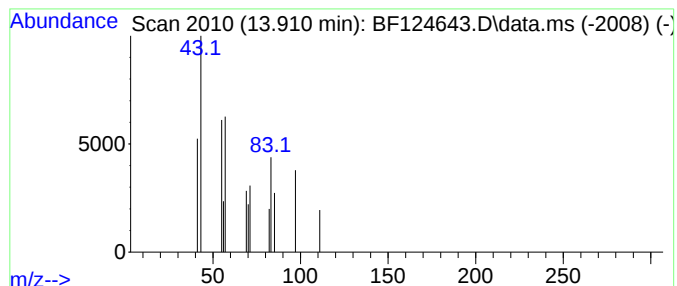
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Peak Number 4 Octadecane, 1-(ethenyloxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	7.09 ng	8350	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	64
2			Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	42
3			Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	42
4			Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	42
5			Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	38



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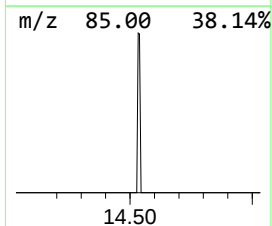
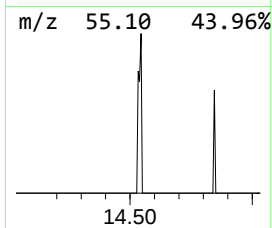
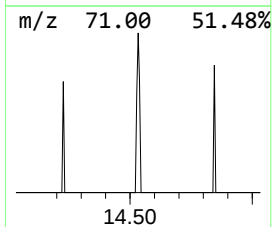
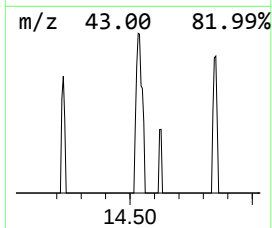
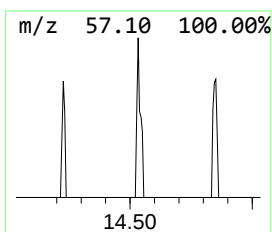
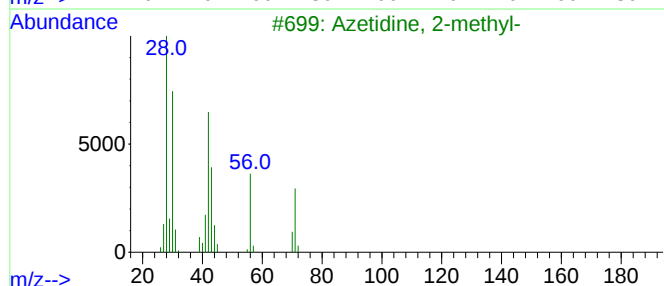
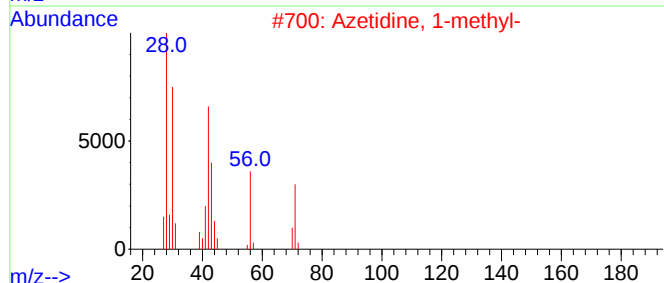
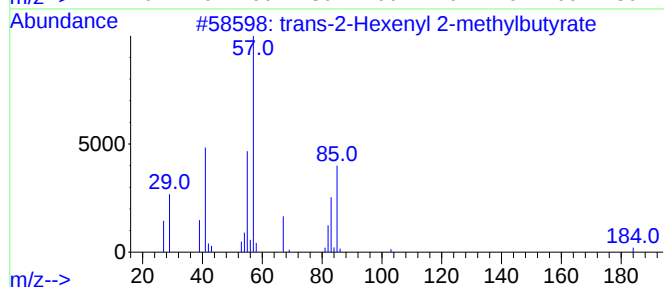
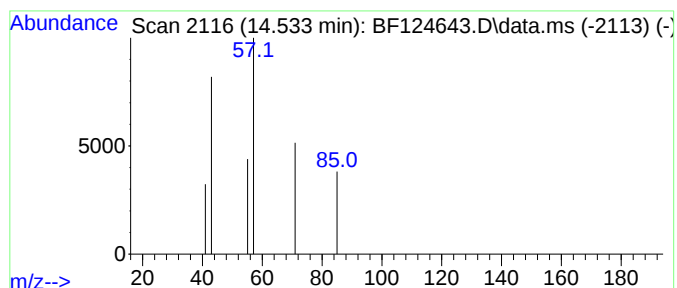
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown14.533 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.533	3.25 ng	3823	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-2-Hexenyl 2-methylbutyrate	184	C11H20O2	1000433-23-8	9
2			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
3			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
4			5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
5			Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	4



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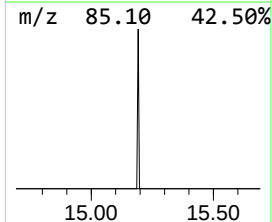
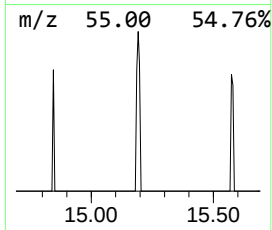
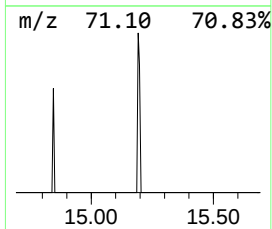
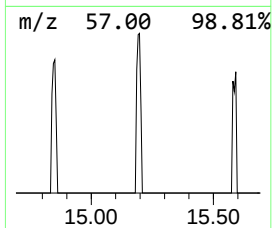
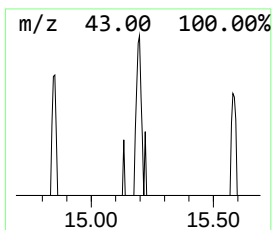
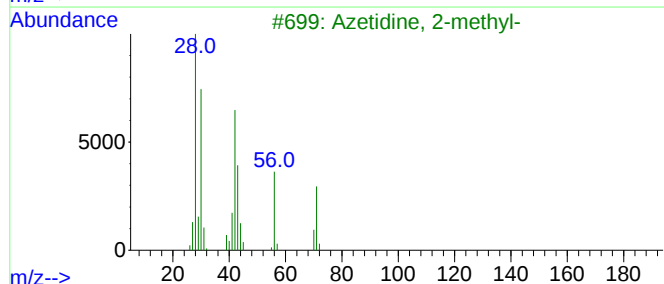
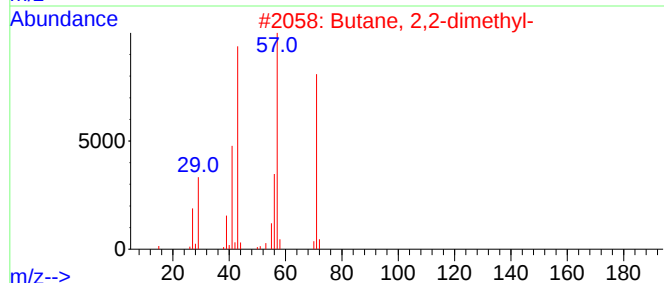
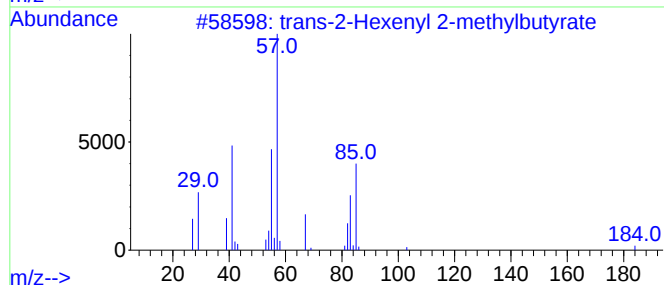
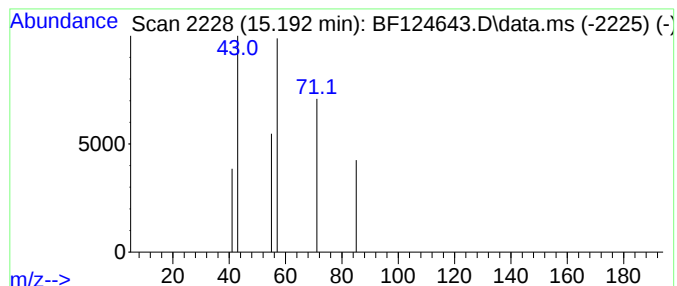
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown15.192 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.192	2.93 ng	3372	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-2-Hexenyl 2-methylbutyrate	184	C11H20O2	1000433-23-8	9
2			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	9
3			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
4			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
5			Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124643.D
Acq On : 20 Jul 2021 23:46
Operator : JU/CG
Sample : M3043-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-077

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.216	4.1	ng	7755	1	6.904	38071	20.0
Ethanol, 2-(2-b...	8.081	5.9	ng	15791	2	8.186	53750	20.0
Dodecanoic acid	11.945	4.5	ng	10735	4	11.427	47562	20.0
Octadecane, 1-(...	13.910	7.1	ng	8350	5	14.068	23546	20.0
unknown14.533	14.533	3.3	ng	3823	5	14.068	23546	20.0
unknown15.192	15.192	2.9	ng	3372	6	15.557	23018	20.0