

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
 Data File : BF124646.D
 Acq On : 21 Jul 2021 1:26
 Operator : JU/CG
 Sample : M3088-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B1-(A-D)-(0-4.5)

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: BF124646.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	19	23	27	rBB	12064	13701	6.33%	1.078%
2	5.145	516	520	523	rBB	2841	3692	1.71%	0.291%
3	5.522	579	584	587	rBB	176880	174602	80.65%	13.740%
4	6.528	749	755	757	rBB	152827	179385	82.86%	14.117%
5	6.904	816	819	822	rBB	51176	37929	17.52%	2.985%
6	7.469	910	915	917	rBB	120668	115142	53.18%	9.061%
7	8.081	1016	1019	1022	rBB	10355	7621	3.52%	0.600%
8	8.186	1033	1037	1040	rBV	68980	50984	23.55%	4.012%
9	9.169	1200	1204	1206	rBV2	1339	2340	1.08%	0.184%
10	9.263	1214	1220	1223	rBV	244333	216502	100.00%	17.038%
11	9.457	1249	1253	1255	rVB3	2354	2689	1.24%	0.212%
12	9.663	1283	1288	1291	rBV2	7060	8873	4.10%	0.698%
13	9.710	1291	1296	1298	rVV3	2591	4683	2.16%	0.369%
14	9.745	1298	1302	1306	rVB4	1790	3376	1.56%	0.266%
15	9.945	1332	1336	1339	rVB	65924	53707	24.81%	4.226%
16	10.057	1353	1355	1357	rBV2	4185	3684	1.70%	0.290%
17	10.239	1382	1386	1389	rBV4	5112	8021	3.70%	0.631%
18	10.286	1392	1394	1396	rBV3	3899	4001	1.85%	0.315%
19	10.316	1397	1399	1401	rVV2	5172	4193	1.94%	0.330%
20	10.592	1441	1446	1449	rBV3	12494	17728	8.19%	1.395%
21	10.686	1460	1462	1465	rVB4	7743	5648	2.61%	0.444%
22	10.733	1466	1470	1473	rVB	119093	98911	45.69%	7.784%
23	11.433	1586	1589	1591	rBV	51481	40175	18.56%	3.162%
24	11.957	1675	1678	1680	rVB2	16628	12771	5.90%	1.005%
25	13.021	1855	1859	1862	rVB	157739	130425	60.24%	10.264%
26	14.051	2032	2034	2035	rBV	22376	13475	6.22%	1.060%
27	14.068	2035	2037	2040	rVB	33578	32143	14.85%	2.529%
28	15.562	2287	2291	2294	rBV	18540	21742	10.04%	1.711%
29	17.051	2542	2544	2549	rVB5	2239	2583	1.19%	0.203%

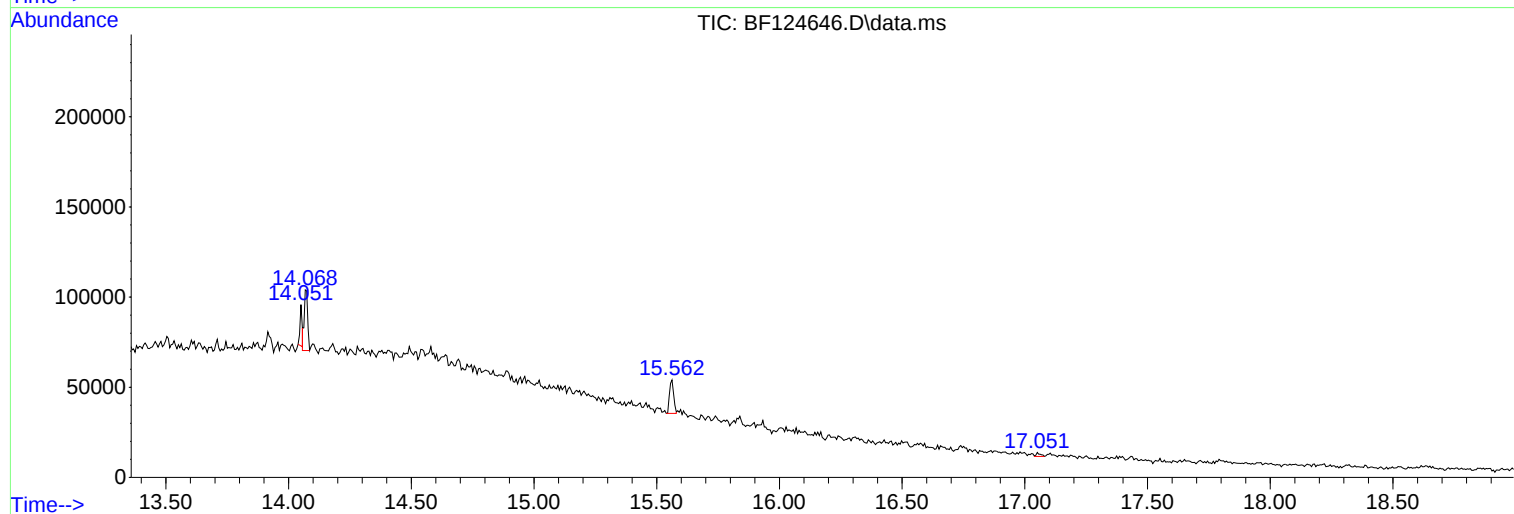
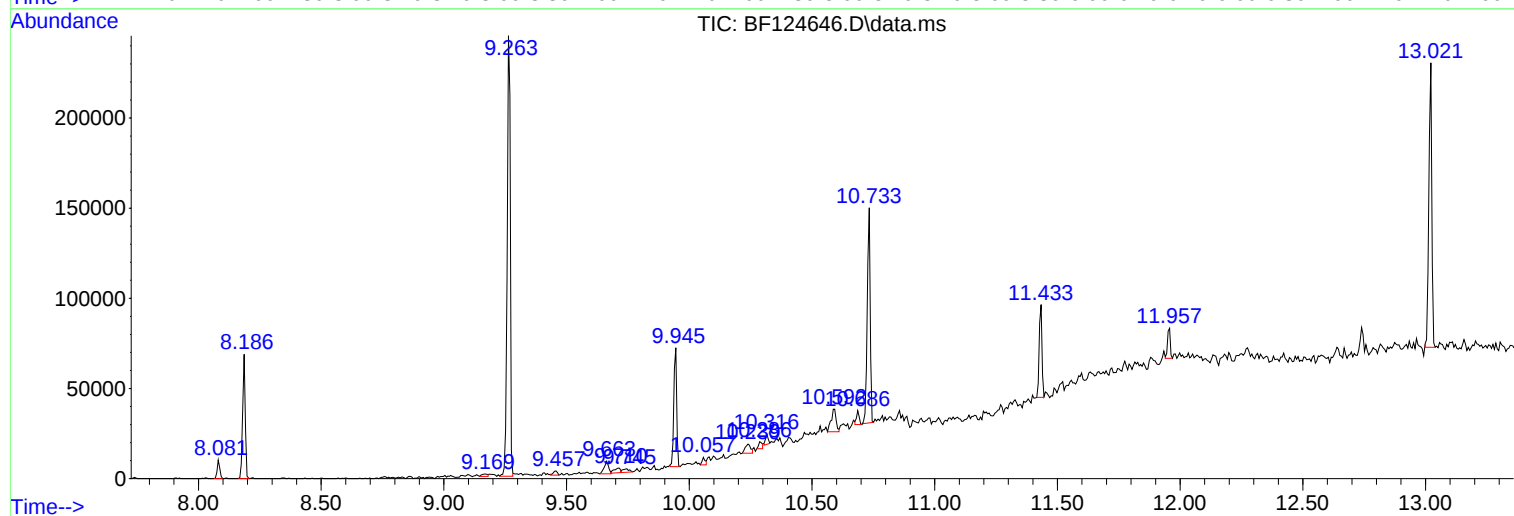
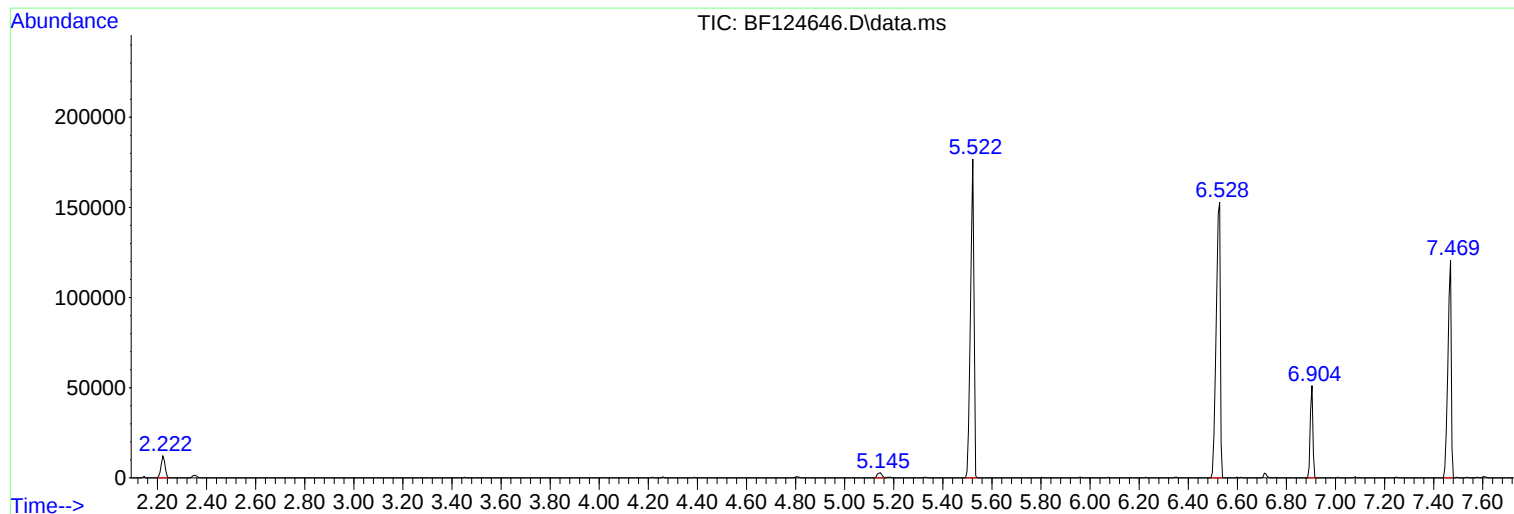
Sum of corrected areas: 1270726

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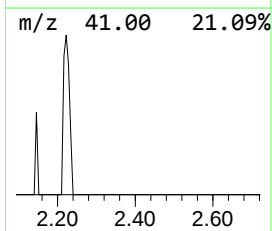
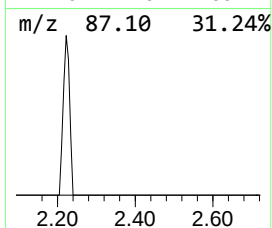
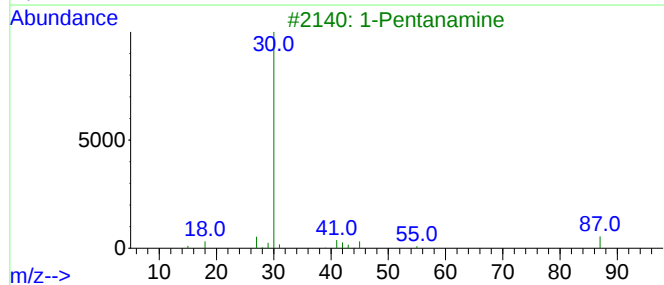
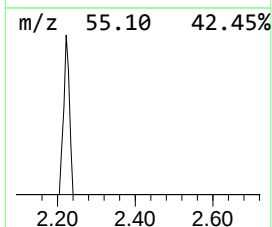
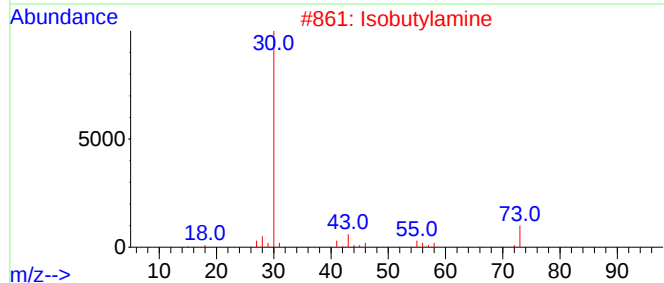
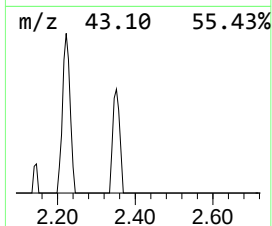
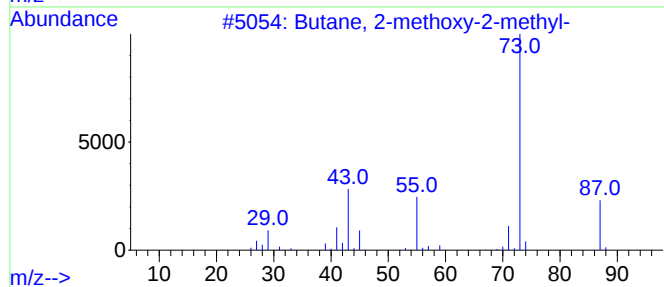
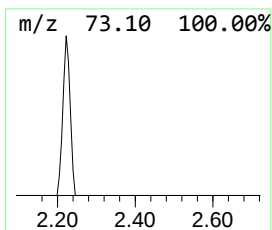
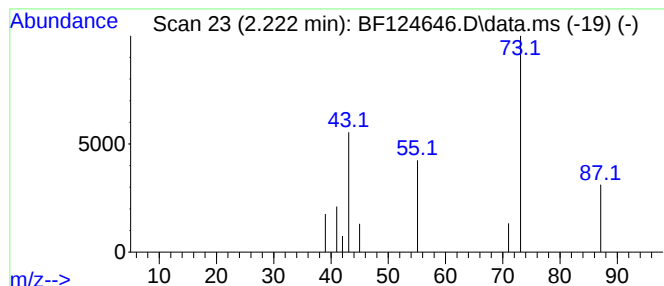
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown2.222 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.222	7.22 ng	13701	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	9
2			Isobutylamine	73	C4H11N	000078-81-9	5
3			1-Pentanamine	87	C5H13N	000110-58-7	4
4			2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	4
5			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	4



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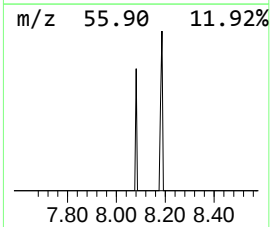
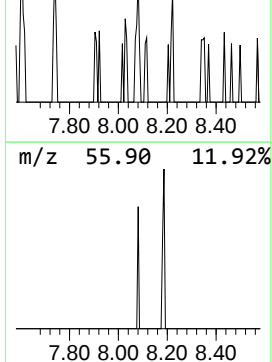
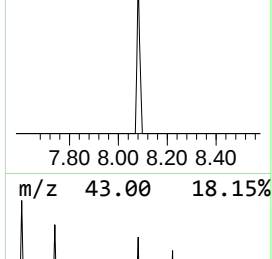
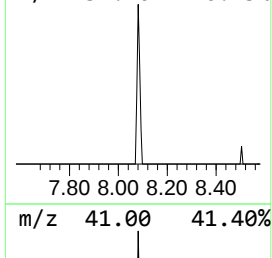
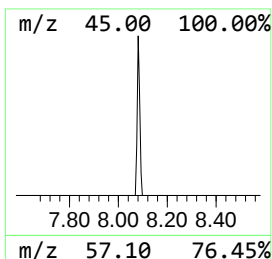
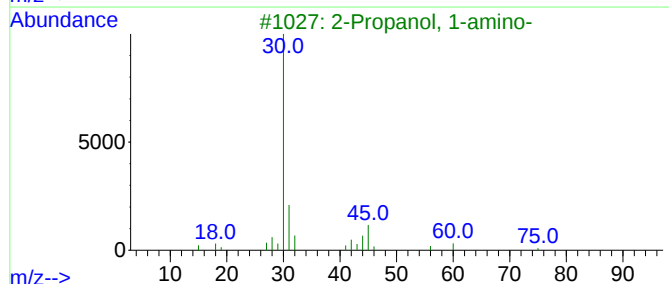
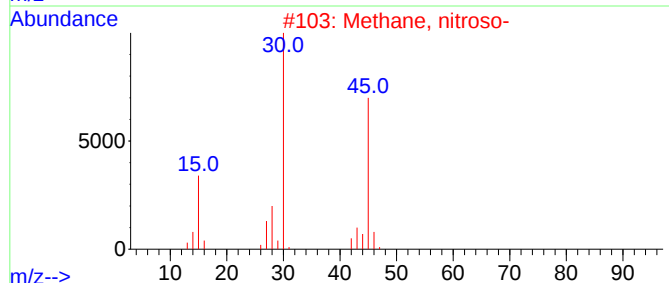
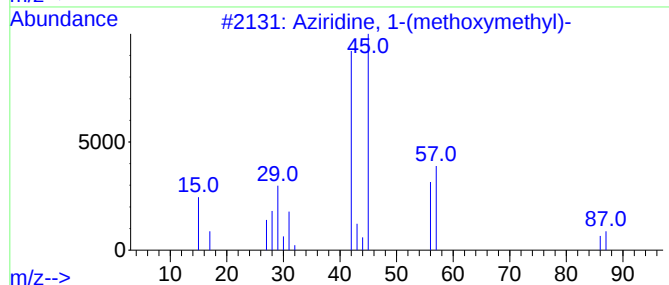
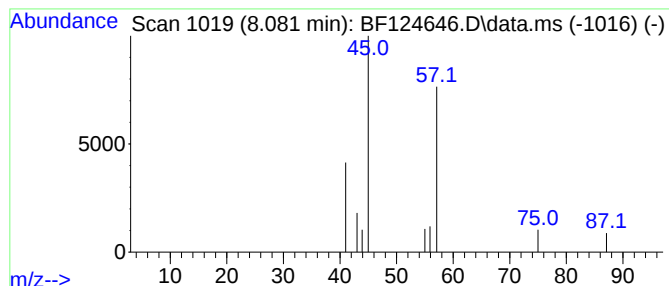
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Peak Number 2 unknown8.081 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.081	2.99 ng	7621	Naphthalene-d8	8.186

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aziridine, 1-(methoxymethyl)-	87	C4H9NO	001497-83-2	7
2			Methane, nitroso-	45	CH3NO	000865-40-7	4
3			2-Propanol, 1-amino-	75	C3H9NO	000078-96-6	4
4			1-Pentanamine	87	C5H13N	000110-58-7	4
5			2-Hexanol	102	C6H14O	000626-93-7	4



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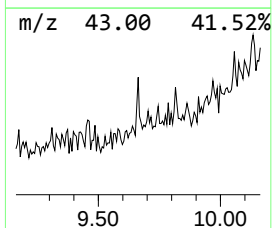
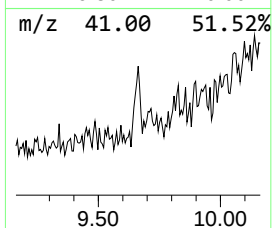
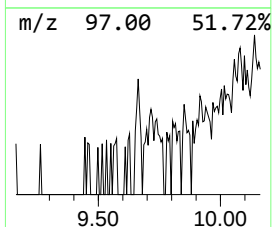
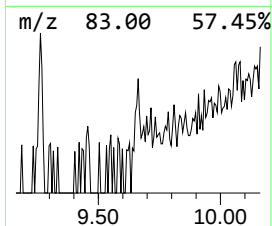
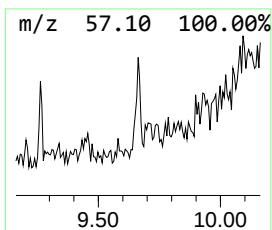
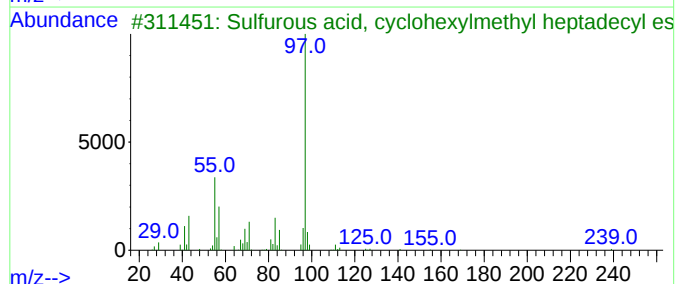
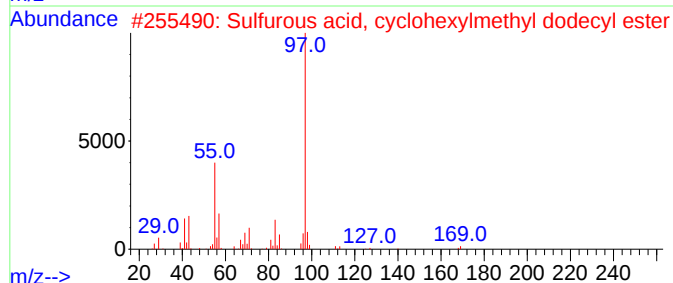
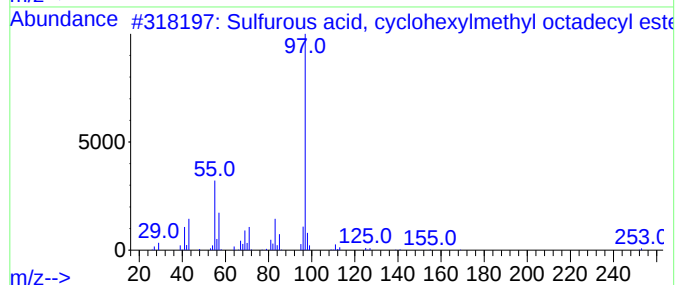
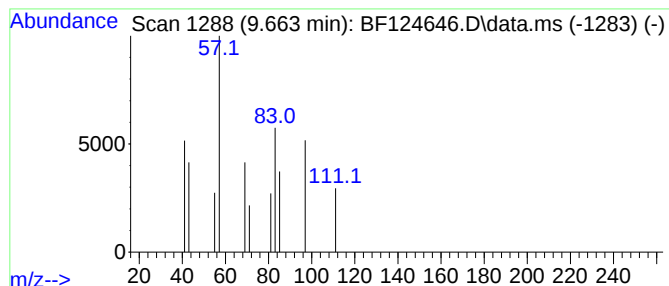
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Peak Number 3 unknown9.663 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.663	3.30 ng	8873	Acenaphthene-d10	9.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, cyclohexylmethyl...	430	C25H50O3S	1000309-22-6	9
2			Sulfurous acid, cyclohexylmethyl...	346	C19H38O3S	1000309-22-0	9
3			Sulfurous acid, cyclohexylmethyl...	416	C24H48O3S	1000309-22-5	9
4			Sulfurous acid, cyclohexylmethyl...	374	C21H42O3S	1000309-22-2	9
5			Sulfurous acid, cyclohexylmethyl...	402	C23H46O3S	1000309-22-4	9



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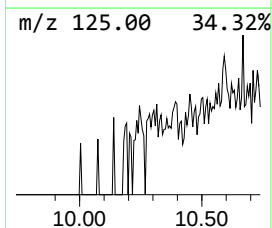
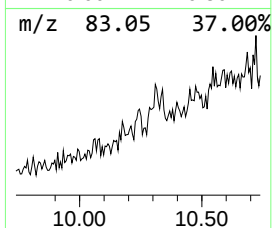
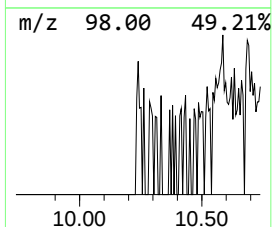
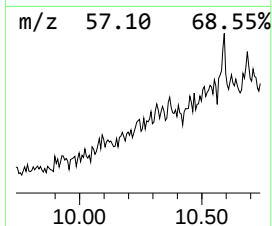
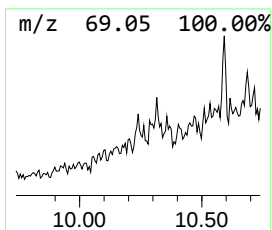
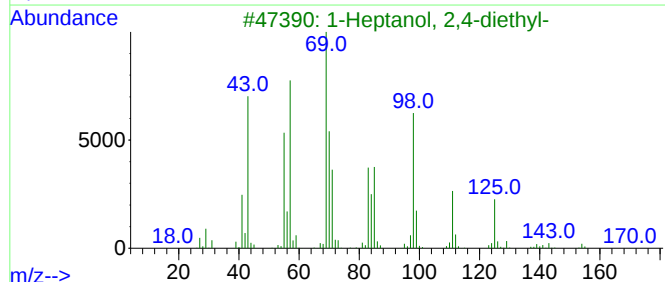
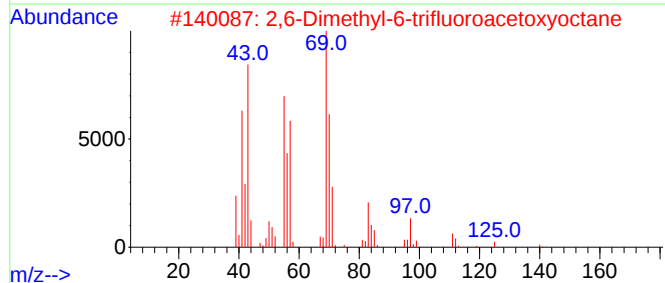
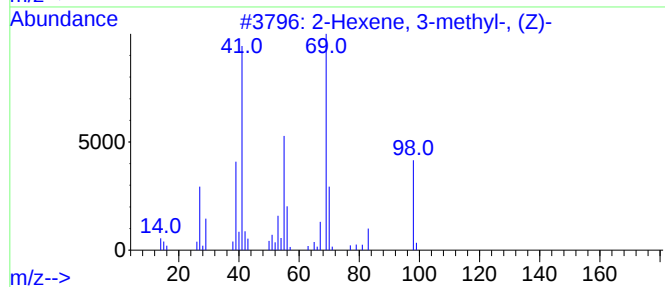
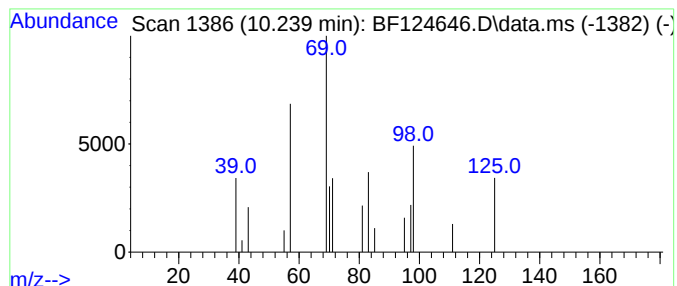
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Peak Number 4 unknown10.239 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.239	2.99 ng	8021	Acenaphthene-d10	9.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexene, 3-methyl-, (Z)-		98	C7H14		010574-36-4	43
2	2,6-Dimethyl-6-trifluoroacetoxy...		254	C12H21F3O2		061986-67-2	40
3	1-Heptanol, 2,4-diethyl-		172	C11H24O		080192-55-8	36
4	Cyclopentane, butyl-		126	C9H18		002040-95-1	28
5	2-Ethyl-1-dodecanol		214	C14H30O		019780-33-7	12



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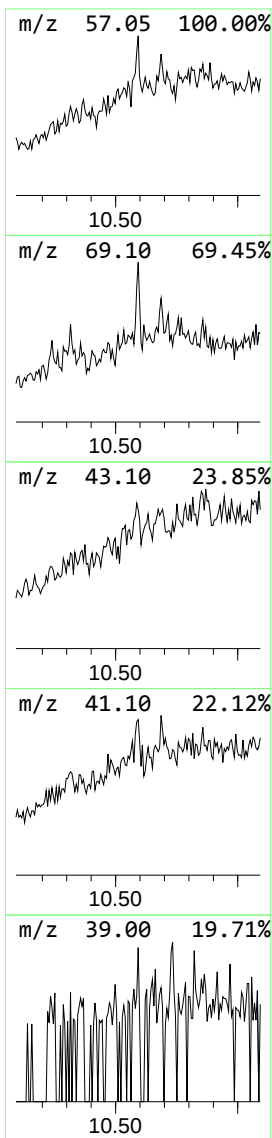
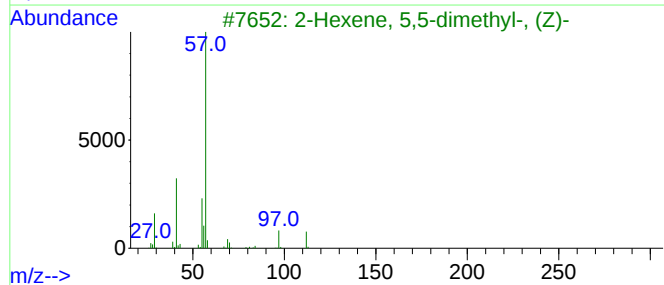
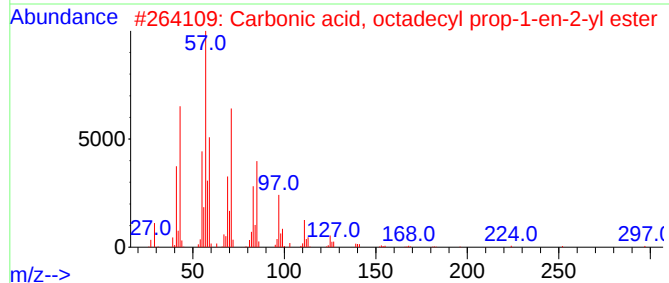
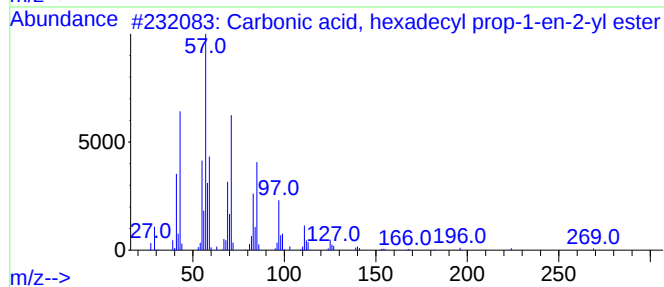
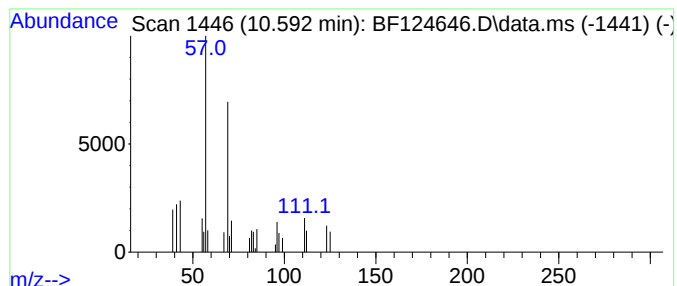
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown10.592 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.592	6.60 ng	17728	Acenaphthene-d10	9.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	40
2			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	37
3			2-Hexene, 5,5-dimethyl-, (Z)-	112	C8H16	039761-61-0	25
4			Heptyl hexadecyl ether	340	C23H48O	1000406-39-4	25
5			Heptyl octacosyl ether	509	C35H72O	1000406-40-0	22



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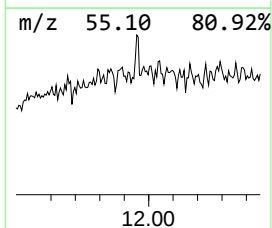
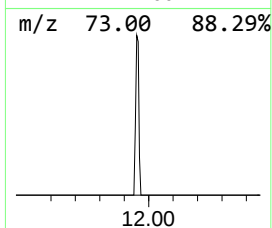
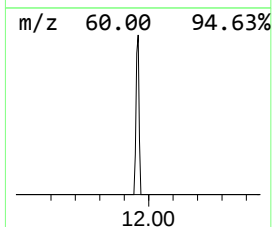
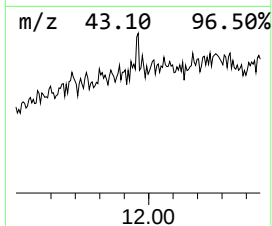
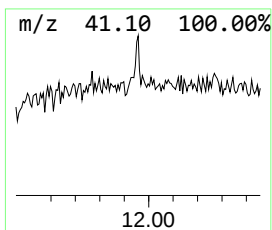
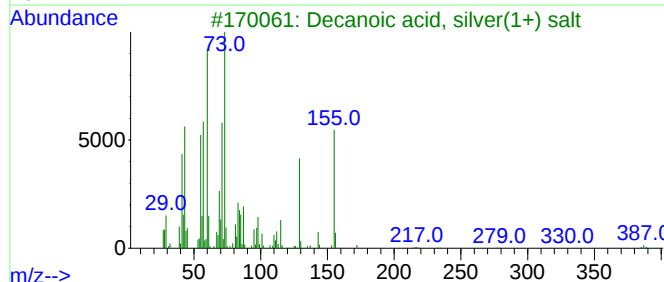
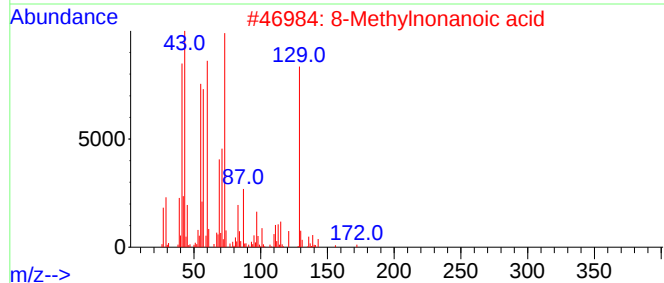
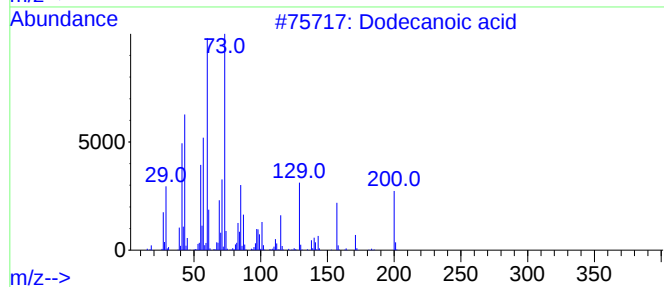
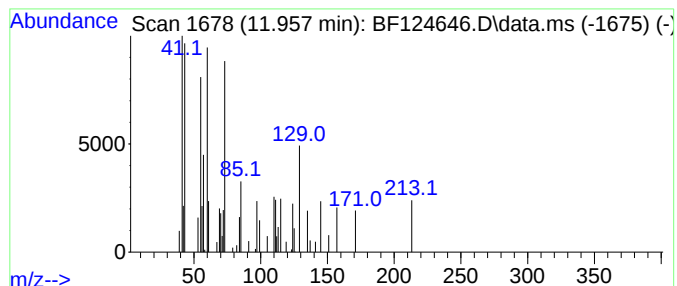
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown11.957 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	6.36 ng	12771	Phenanthrene-d10	11.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	32
2			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	25
3			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	17
4			n-Decanoic acid	172	C10H20O2	000334-48-5	17
5			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124646.D
Acq On : 21 Jul 2021 1:26
Operator : JU/CG
Sample : M3088-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B1-(A-D)-(0-4.5)

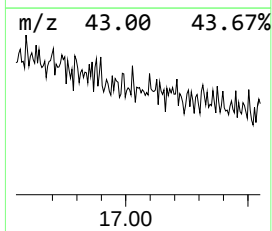
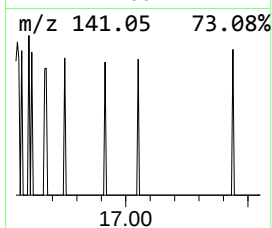
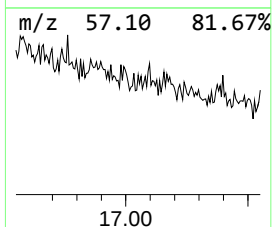
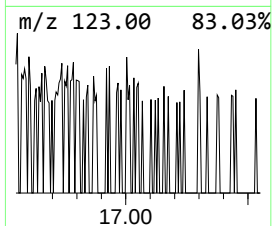
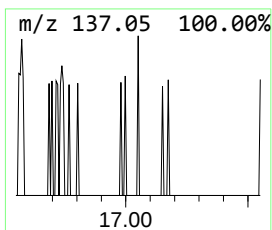
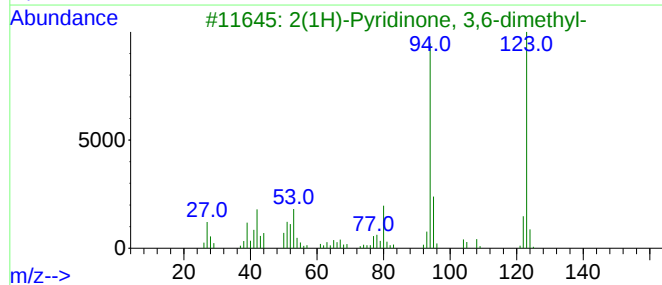
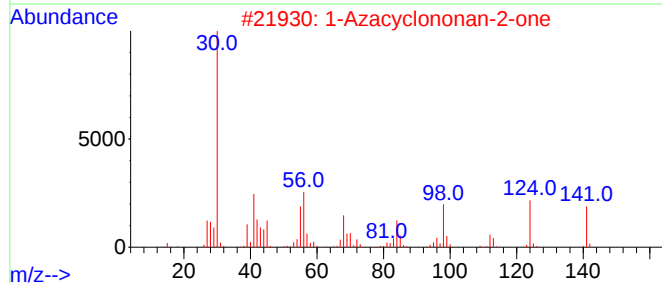
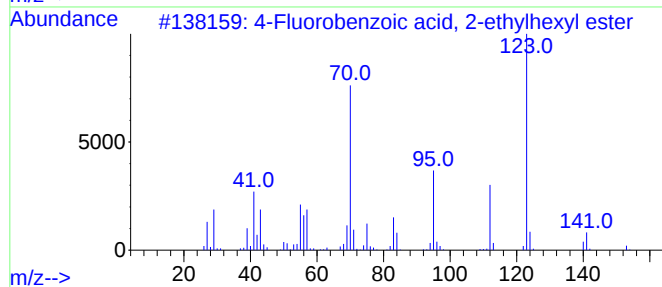
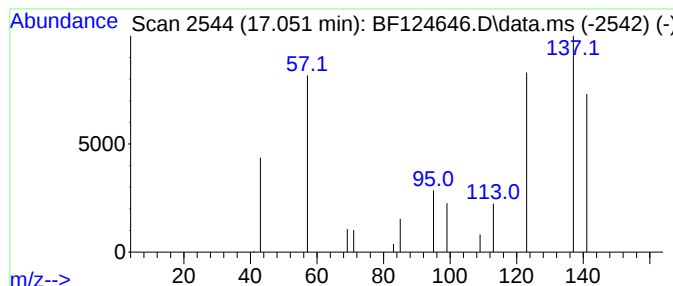
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown17.051 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.051	2.38 ng	2583	Perylene-d12	15.562

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Fluorobenzoic acid, 2-ethylhex...	252	C15H21FO2	059986-38-8	9
2		1-Azacyclononan-2-one	141	C8H15NO	000935-30-8	5
3		2(1H)-Pyridinone, 3,6-dimethyl-	123	C7H9NO	053428-02-7	5
4		Benzene-1,2,3-triamine	123	C6H9N3	1000316-45-3	5
5		N2-Methyl-2,3-pyridinediamine	123	C6H9N3	005028-20-6	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124646.D
Acq On : 21 Jul 2021 1:26
Operator : JU/CG
Sample : M3088-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B1-(A-D)-(0-4.5)

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
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unknown8.081	8.081	3.0	ng	7621	2	8.186	50984	20.0
unknown9.663	9.663	3.3	ng	8873	3	9.945	53707	20.0
unknown10.239	10.239	3.0	ng	8021	3	9.945	53707	20.0
unknown10.592	10.592	6.6	ng	17728	3	9.945	53707	20.0
unknown11.957	11.957	6.4	ng	12771	4	11.433	40175	20.0
unknown17.051	17.051	2.4	ng	2583	6	15.562	21742	20.0