

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072221\
 Data File : BF124702.D
 Acq On : 22 Jul 2021 22:10
 Operator : JU/CG
 Sample : M3093-04
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20210537-COM-10

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: BF124702.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	8	12	15	rBB	13575	15942	7.81%	1.299%
2	5.098	509	512	516	rBB	2562	2869	1.40%	0.234%
3	5.487	573	578	580	rBB	168921	166257	81.40%	13.552%
4	6.492	743	749	752	rBV	167658	171192	83.81%	13.954%
5	6.869	810	813	816	rBB	41645	29120	14.26%	2.374%
6	7.434	904	909	911	rBB	121763	109124	53.43%	8.895%
7	8.051	1011	1014	1016	rBB	12955	9483	4.64%	0.773%
8	8.151	1027	1031	1034	rBB	55308	42065	20.59%	3.429%
9	9.228	1210	1214	1217	rBB	247578	204251	100.00%	16.649%
10	9.904	1326	1329	1332	rBB	60861	47635	23.32%	3.883%
11	10.692	1460	1463	1466	rBB	136537	129869	63.58%	10.586%
12	11.392	1579	1582	1585	rBV	61594	45293	22.18%	3.692%
13	11.916	1668	1671	1673	rBB	16241	11825	5.79%	0.964%
14	12.698	1802	1804	1806	rBB	4638	2715	1.33%	0.221%
15	12.980	1848	1852	1855	rBB	213095	180977	88.61%	14.752%
16	14.027	2026	2030	2033	rBV	35637	28431	13.92%	2.318%
17	14.880	2173	2175	2178	rBB	3021	2661	1.30%	0.217%
18	15.498	2276	2280	2284	rBB	25805	27083	13.26%	2.208%

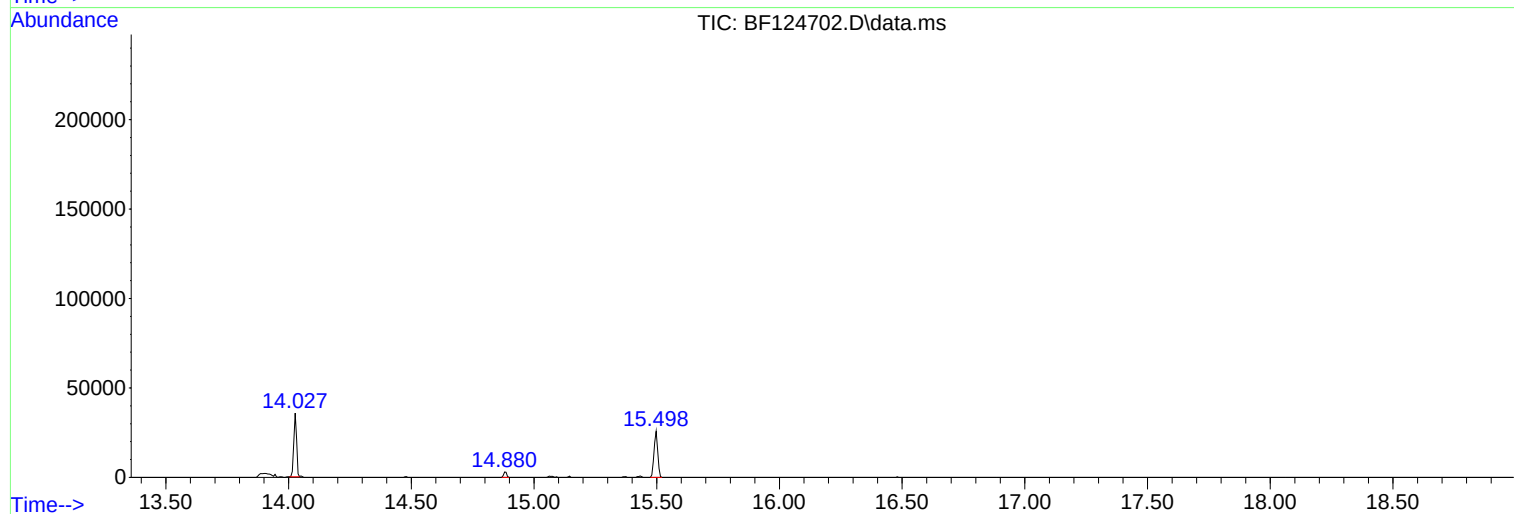
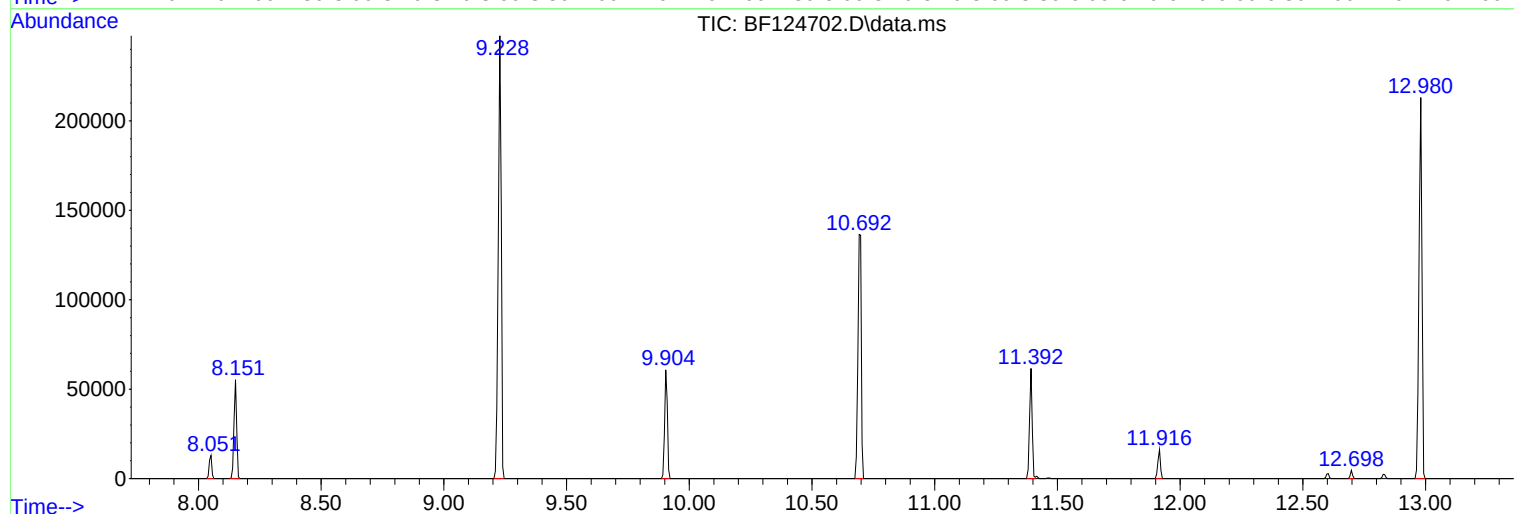
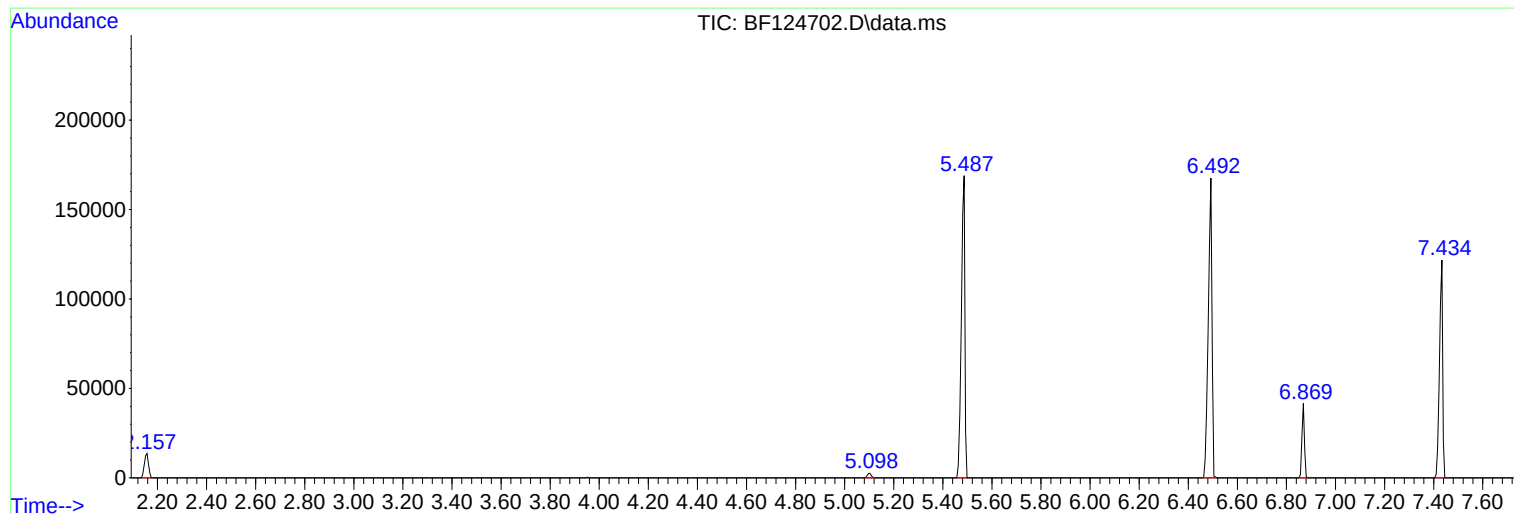
Sum of corrected areas: 1226792

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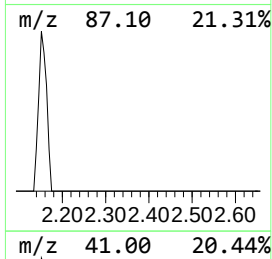
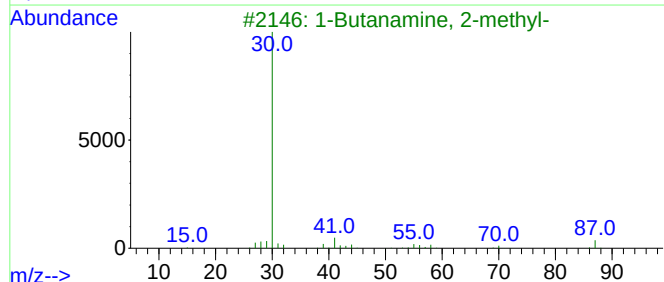
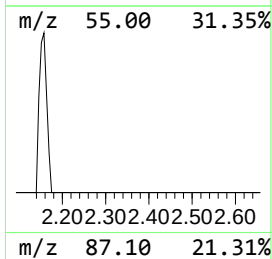
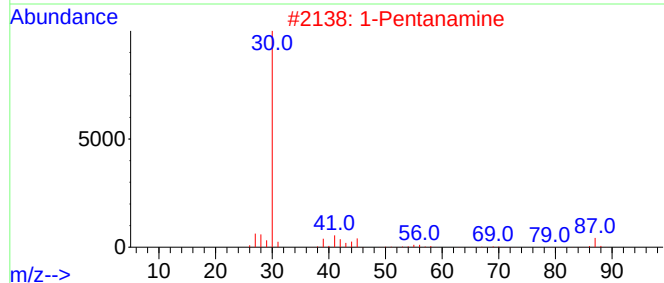
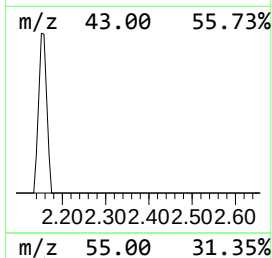
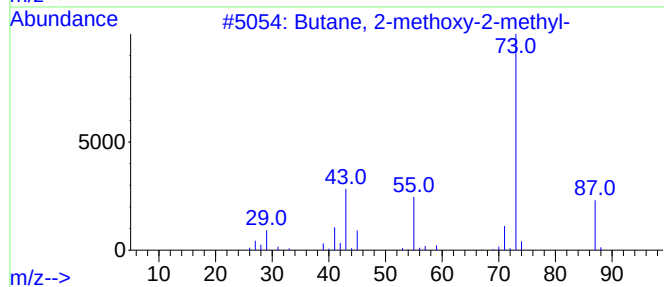
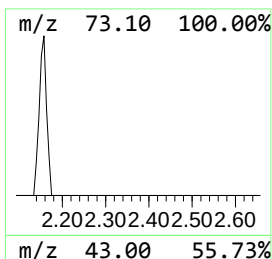
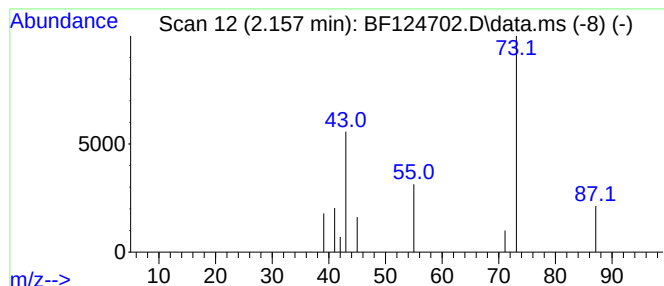
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	10.95 ng	15942	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	74
2			1-Pentanamine	87	C5H13N	000110-58-7	7
3			1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	4
4			Isobutylamine	73	C4H11N	000078-81-9	4
5			2-OXOPROPIONAMIDE	87	C3H5NO2	000631-66-3	4



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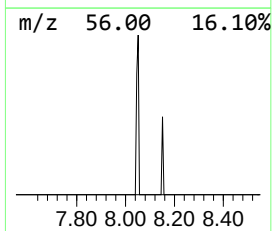
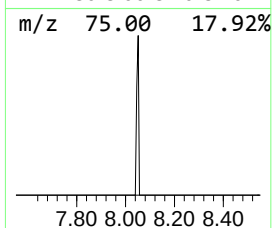
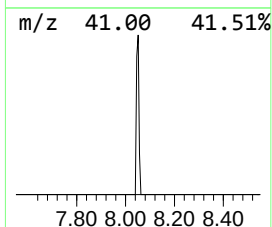
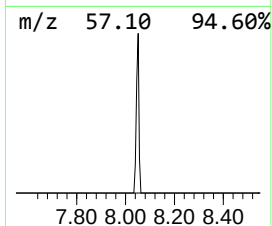
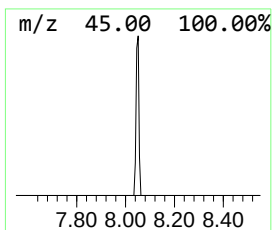
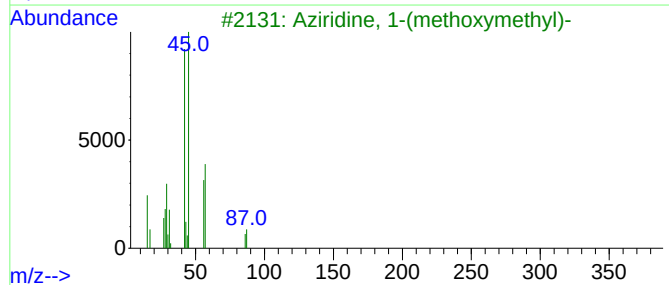
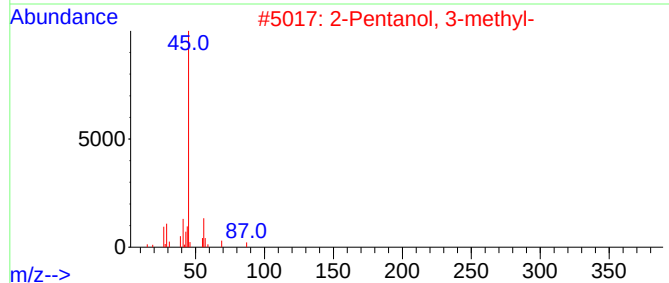
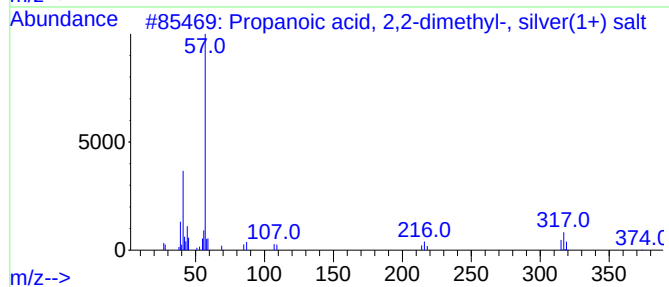
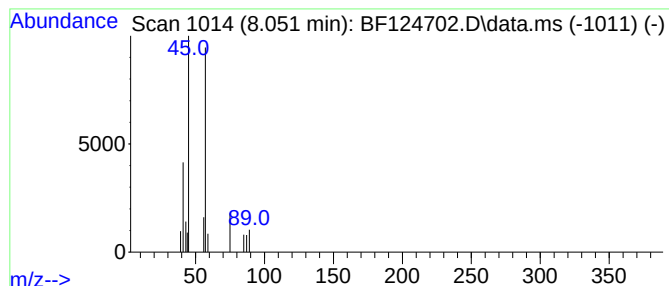
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Peak Number 2 unknown8.051 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	4.51 ng	9483	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	9
2			2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	9
3			Aziridine, 1-(methoxymethyl)-	87	C4H9NO	001497-83-2	7
4			4-Amino-1-butanol	89	C4H11NO	013325-10-5	5
5			Methane, nitroso-	45	CH3NO	000865-40-7	4



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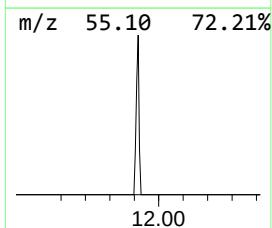
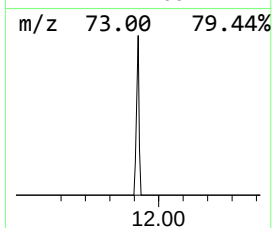
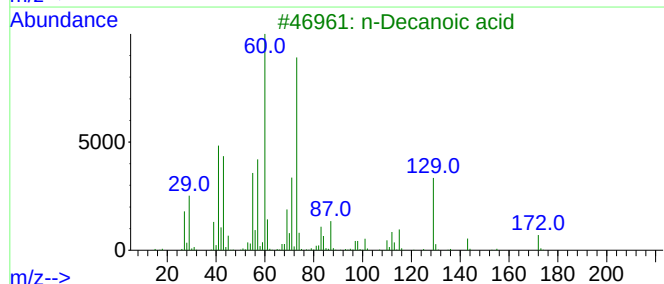
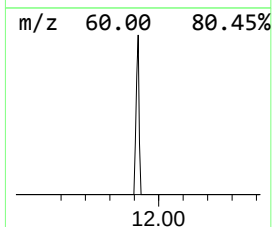
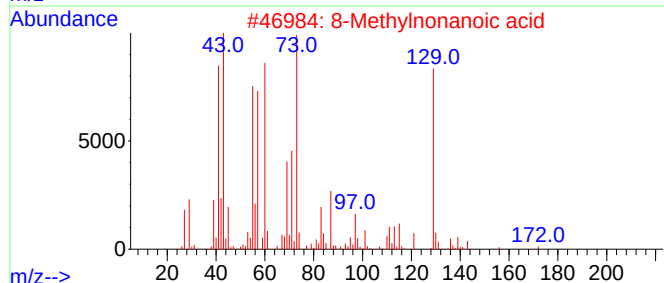
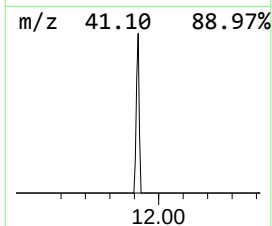
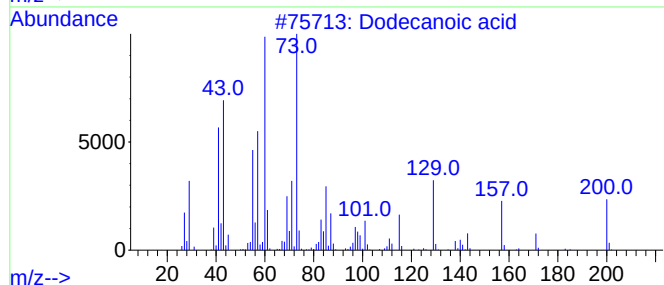
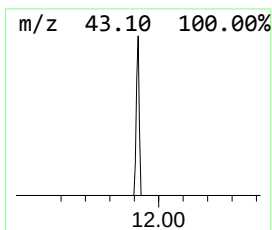
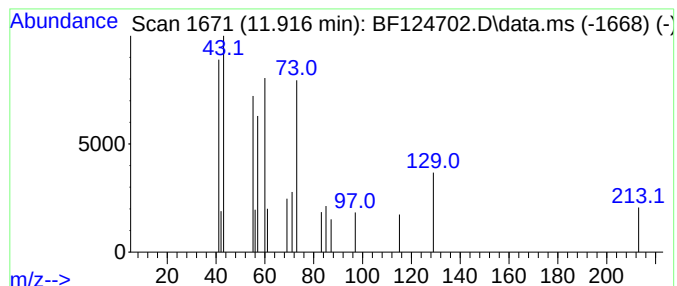
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Peak Number 3 Dodecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.916	5.22 ng	11825	Phenanthrene-d10	11.392	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	64
2	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	53
3	n-Decanoic acid	172	C10H20O2	000334-48-5	50
4	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	50
5	.beta.-d-Lyxofuranoside, thio-de...	306	C15H30O4S	1000154-40-2	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.157	10.9	ng	15942	1	6.869	29120	20.0
unknown8.051	8.051	4.5	ng	9483	2	8.151	42065	20.0
Dodecanoic acid	11.916	5.2	ng	11825	4	11.392	45293	20.0