

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
 Data File : BF124191.D
 Acq On : 8 Jun 2021 21:17
 Operator : JU/CG
 Sample : M2629-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OK-02-060721

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-BF060321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124191.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	4	10	19	rVB	435426	566896	49.20%	6.266%
2	2.257	24	29	34	rBV	18745	23379	2.03%	0.258%
3	2.975	146	151	156	rVB2	10380	15059	1.31%	0.166%
4	5.087	506	510	515	rVB	31252	36096	3.13%	0.399%
5	5.498	576	580	591	rBV	958747	883605	76.69%	9.766%
6	6.510	747	752	759	rBV	831508	874978	75.94%	9.671%
7	6.863	808	812	815	rBB	335229	263030	22.83%	2.907%
8	7.428	903	908	911	rBV	621333	616238	53.49%	6.811%
9	8.145	1026	1030	1033	rBV	397896	310034	26.91%	3.427%
10	9.222	1208	1213	1216	rBV	1417414	1152162	100.00%	12.734%
11	9.898	1324	1328	1332	rBV	404199	325222	28.23%	3.594%
12	10.692	1459	1463	1466	rBV	644620	596871	51.80%	6.597%
13	11.245	1551	1557	1561	rBV3	8833	14224	1.23%	0.157%
14	11.386	1577	1581	1583	rBV	321866	265633	23.06%	2.936%
15	11.410	1583	1585	1588	rVB	83411	59036	5.12%	0.652%
16	11.774	1644	1647	1651	rVB2	24423	20210	1.75%	0.223%
17	11.998	1684	1685	1693	rVB4	14761	17785	1.54%	0.197%
18	12.486	1763	1768	1771	rBV5	20655	25415	2.21%	0.281%
19	12.598	1784	1787	1793	rVB	100923	94727	8.22%	1.047%
20	12.792	1817	1820	1822	rBV	75391	61408	5.33%	0.679%
21	12.833	1822	1827	1831	rVB	78903	91738	7.96%	1.014%
22	12.974	1847	1851	1854	rBV	1066315	888438	77.11%	9.819%
23	13.157	1879	1882	1885	rVB5	15892	19444	1.69%	0.215%
24	13.468	1931	1935	1939	rBV	531754	417662	36.25%	4.616%
25	13.527	1942	1945	1949	rBV	73557	64288	5.58%	0.711%
26	13.827	1994	1996	1998	rBV3	17770	14308	1.24%	0.158%
27	13.892	2006	2007	2010	rBV3	22575	19229	1.67%	0.213%
28	14.033	2024	2031	2033	rBV	298372	323942	28.12%	3.580%
29	14.057	2033	2035	2039	rVB	40560	42753	3.71%	0.473%
30	14.798	2157	2161	2166	rBV	416159	459600	39.89%	5.080%
31	15.074	2206	2208	2213	rBV2	34047	57616	5.00%	0.637%
32	15.386	2259	2261	2265	rVB4	31667	25912	2.25%	0.286%
33	15.451	2269	2272	2277	rVB4	26369	36414	3.16%	0.402%
34	15.515	2279	2283	2288	rVV	189426	229438	19.91%	2.536%
35	16.480	2446	2447	2450	rBV3	15947	17961	1.56%	0.199%
36	16.992	2531	2534	2535	rBV3	15006	20187	1.75%	0.223%

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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

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37	17.080	2547	2549	2554	rVB6	16757	25372	2.20%	0.280%
38	17.251	2574	2578	2583	rBV8	16363	27448	2.38%	0.303%
39	17.450	2607	2612	2616	rBV8	13833	30111	2.61%	0.333%
40	18.450	2780	2782	2784	rBV3	12330	14024	1.22%	0.155%

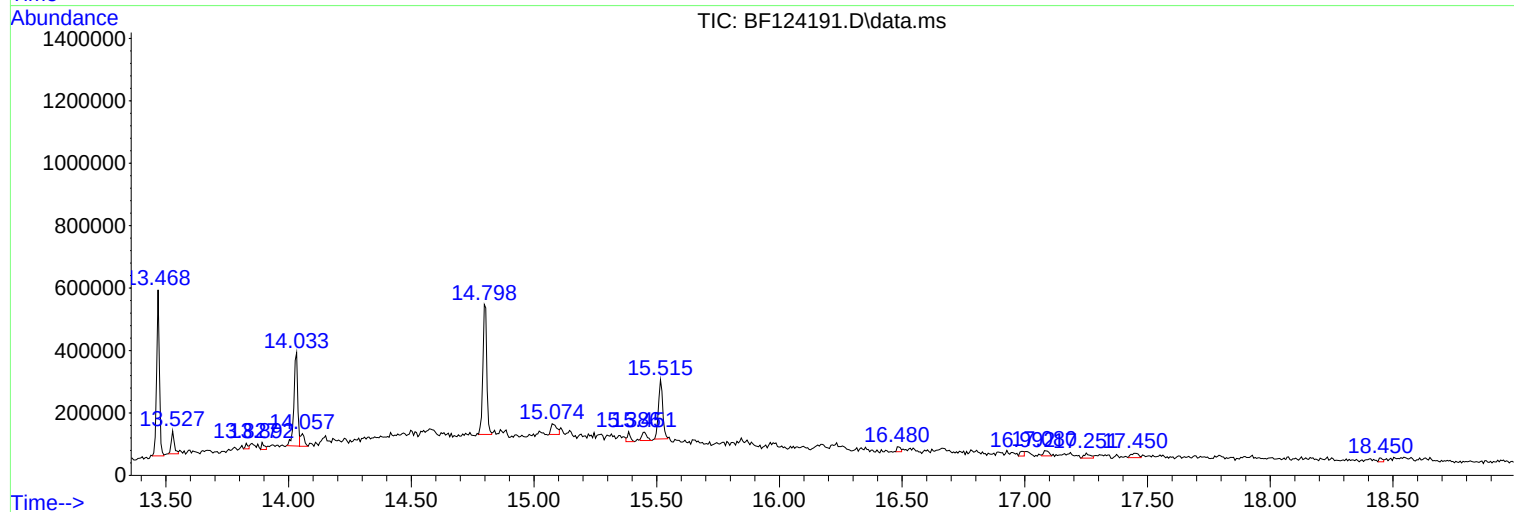
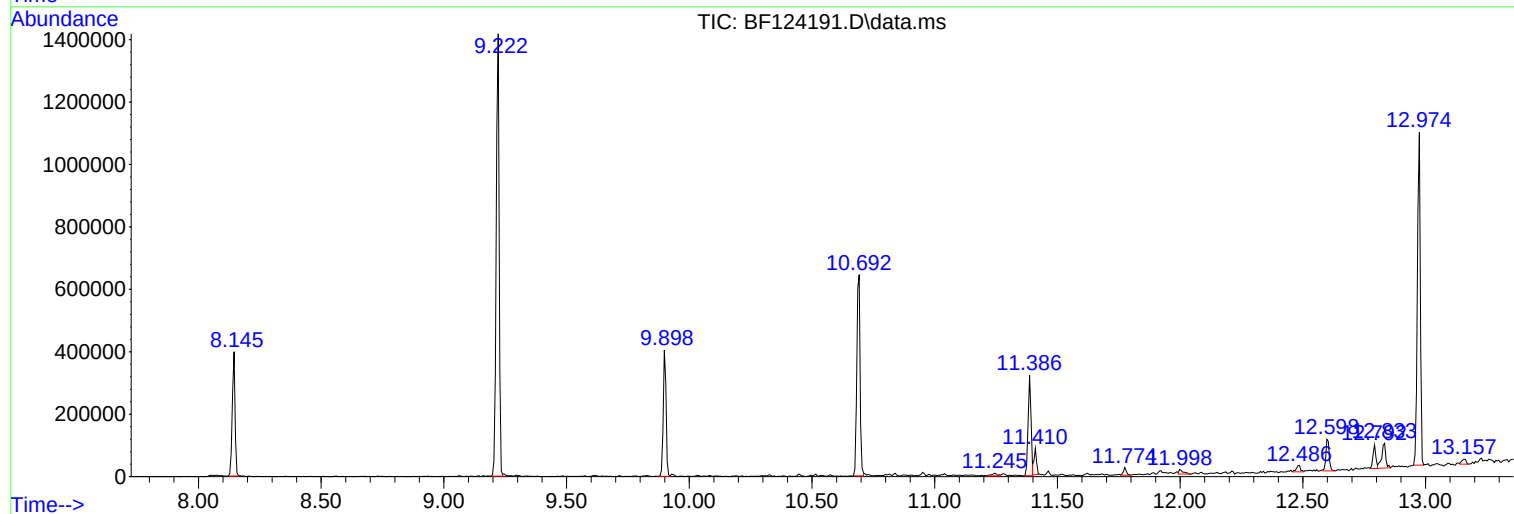
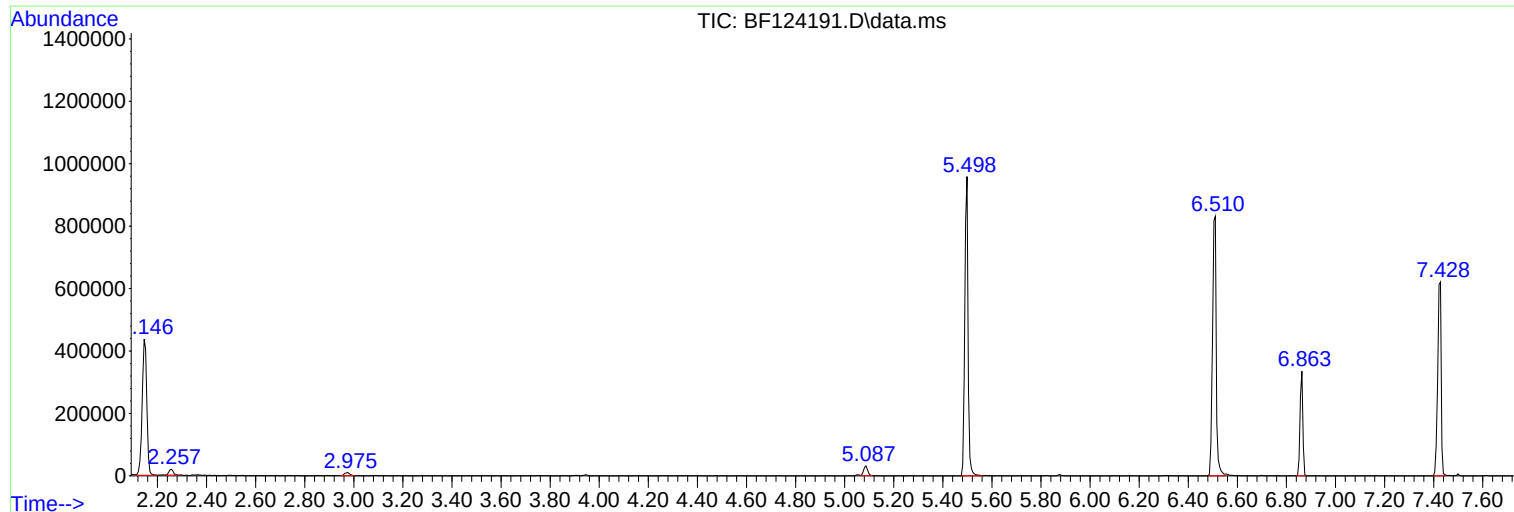
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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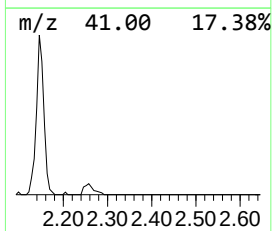
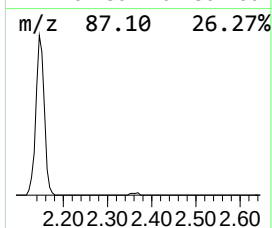
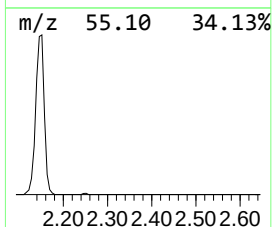
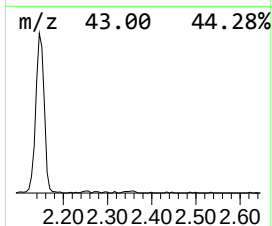
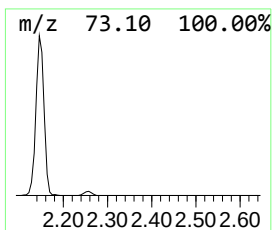
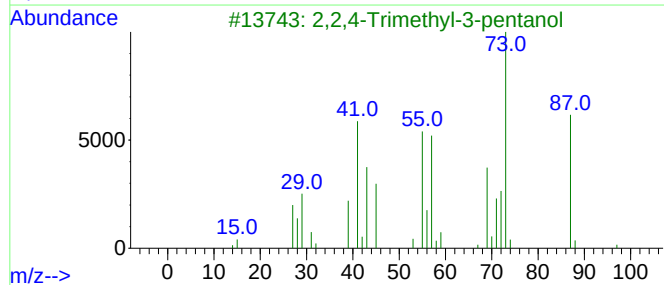
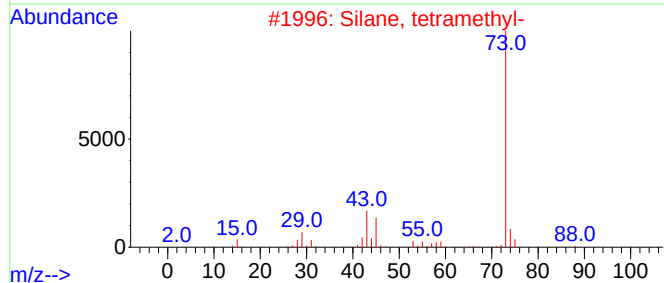
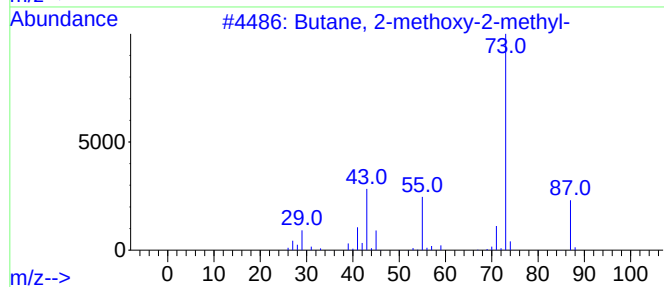
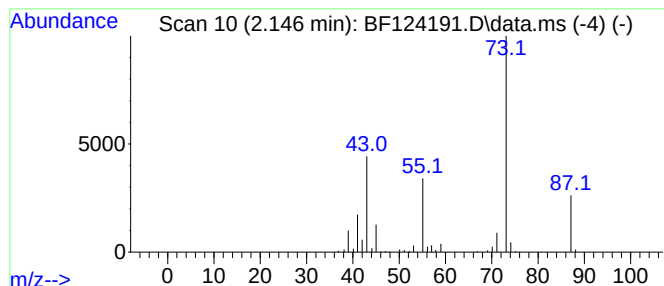
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	43.10 ng	566896	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			Propane, 1-ethoxy-	88	C5H12O	000628-32-0	9



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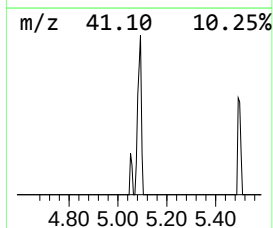
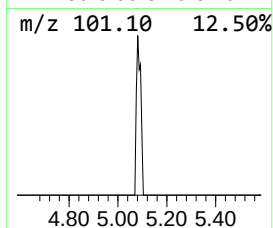
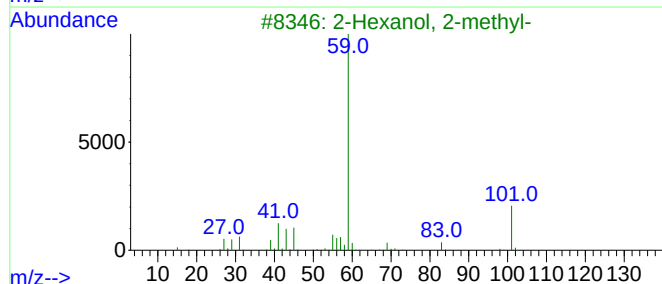
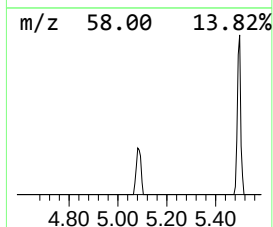
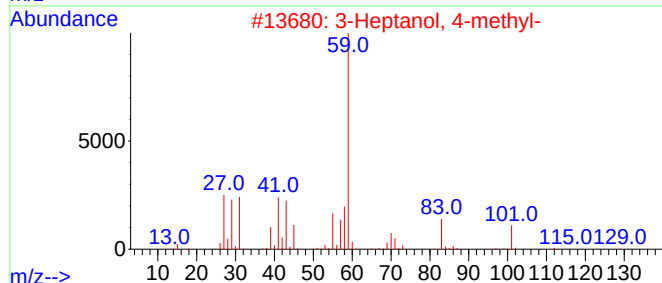
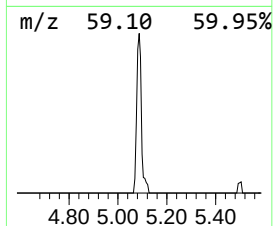
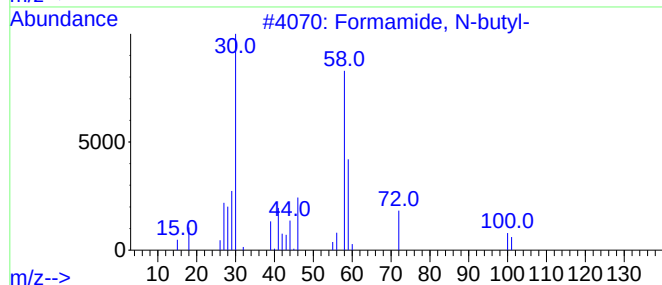
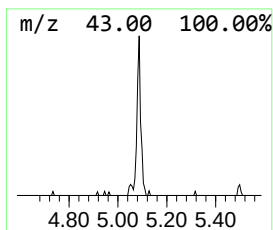
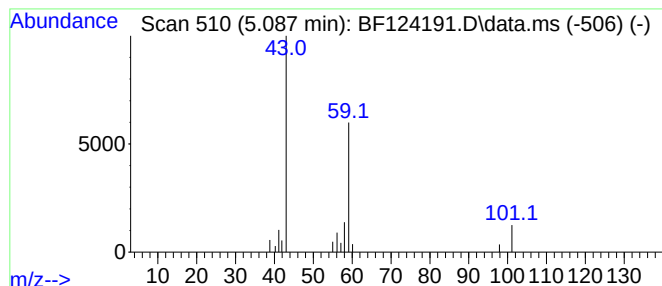
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.087 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	2.74 ng	36096	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Formamide, N-butyl-	101	C5H11NO	000871-71-6	38
2			3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	28
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4			Diacetamide	101	C4H7NO2	000625-77-4	9
5			1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	9



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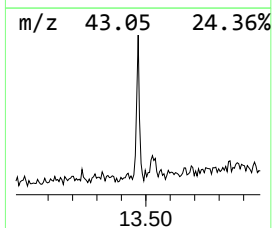
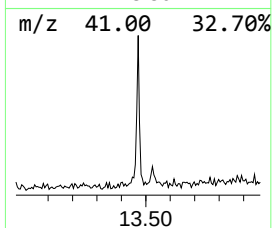
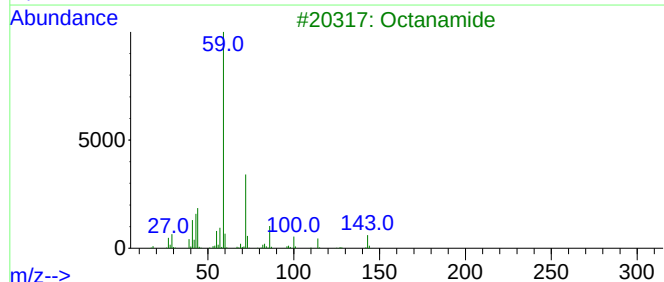
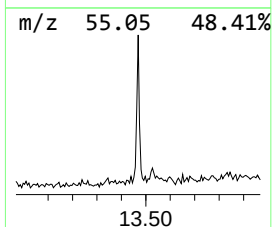
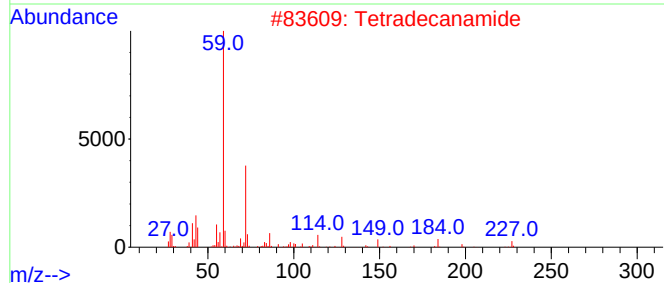
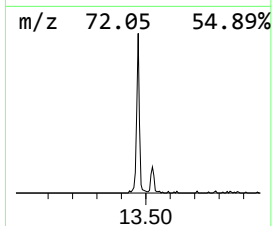
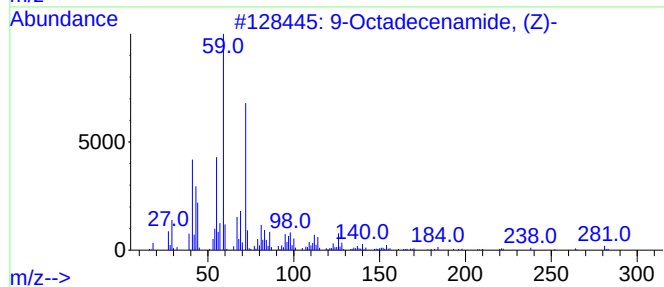
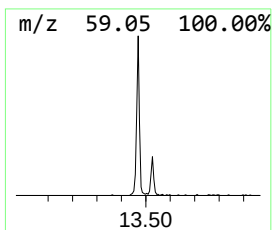
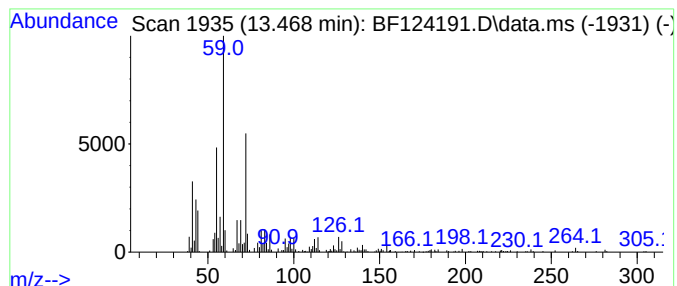
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.468	25.79 ng	417662	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2			Tetradecanamide	227	C14H29NO	000638-58-4	72
3			Octanamide	143	C8H17NO	000629-01-6	64
4			7-Nonenamide	155	C9H17NO	090949-53-4	59
5			Dodecanamide	199	C12H25NO	001120-16-7	59



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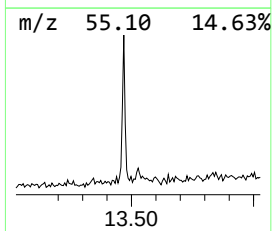
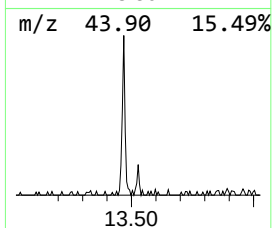
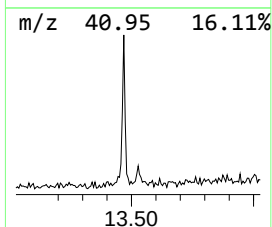
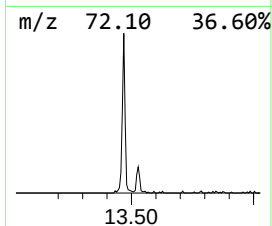
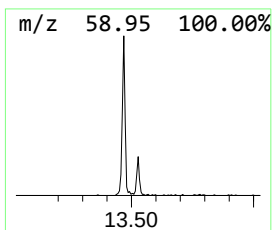
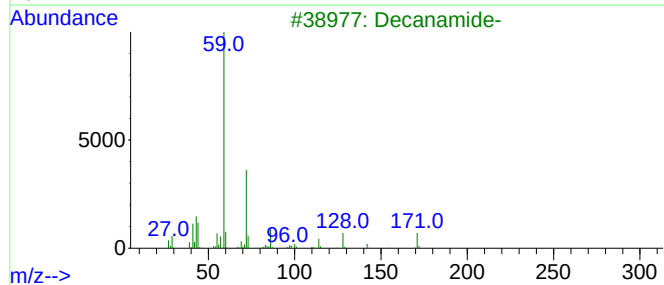
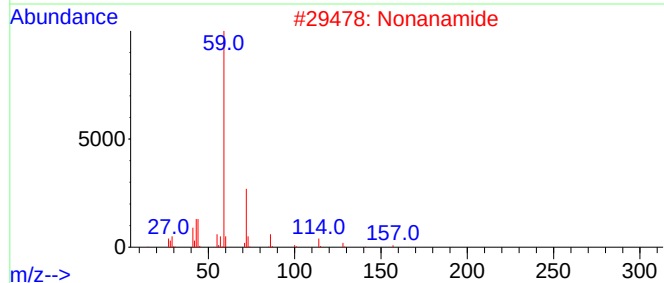
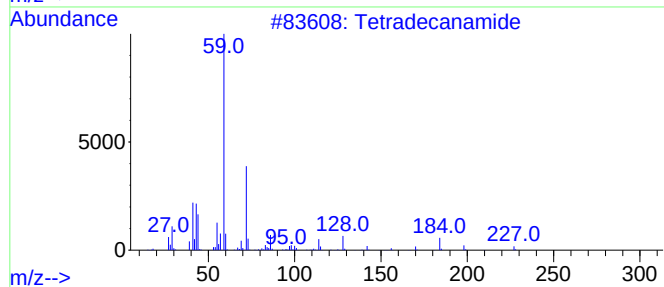
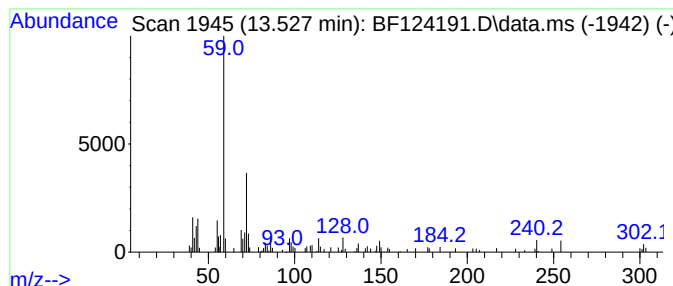
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetradecanamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.527	3.97 ng	64288	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanamide	227	C14H29NO	000638-58-4	64
2			Nonanamide	157	C9H19NO	001120-07-6	64
3			Decanamide-	171	C10H21NO	002319-29-1	64
4			Dodecanamide	199	C12H25NO	001120-16-7	64
5			Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	64



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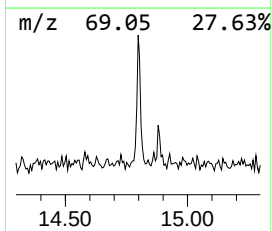
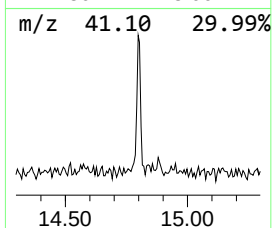
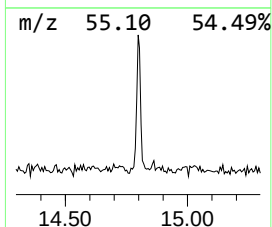
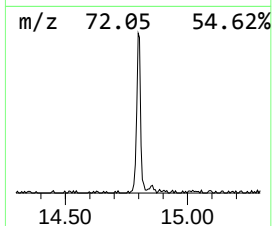
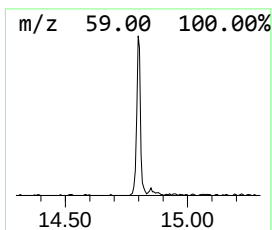
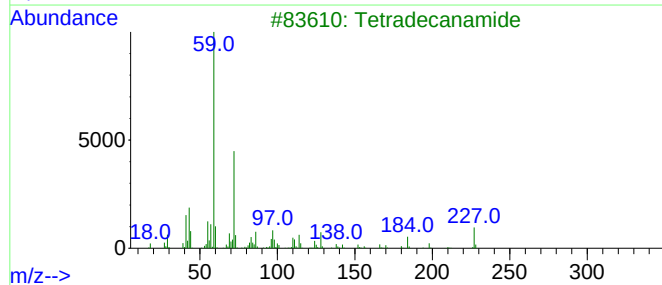
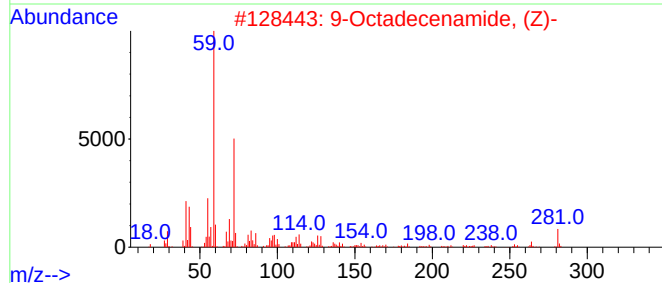
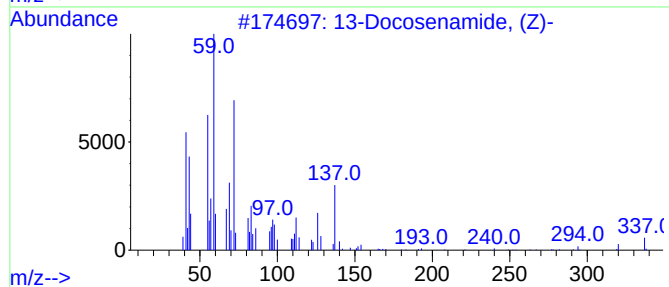
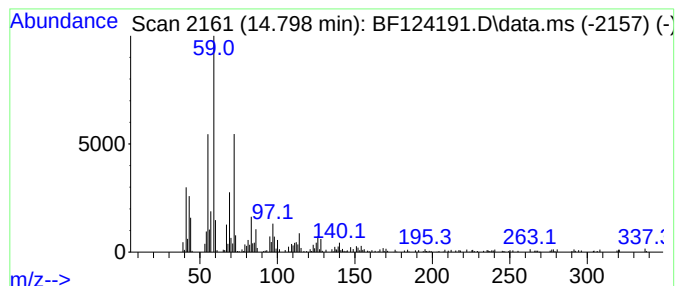
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.798	40.06 ng	459600	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
3			Tetradecanamide	227	C14H29NO	000638-58-4	78
4			Hexadecanamide	255	C16H33NO	000629-54-9	78
5			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
Data File : BF124191.D
Acq On : 8 Jun 2021 21:17
Operator : JU/CG
Sample : M2629-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OK-02-060721

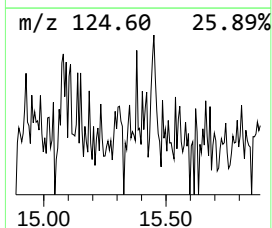
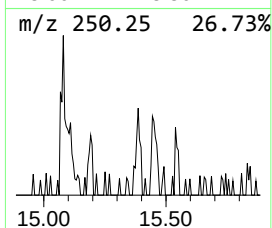
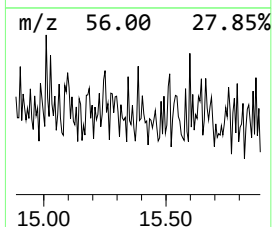
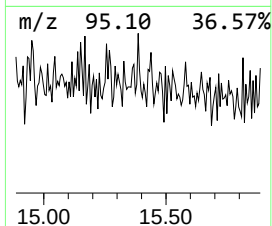
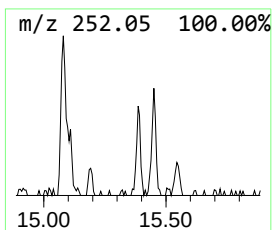
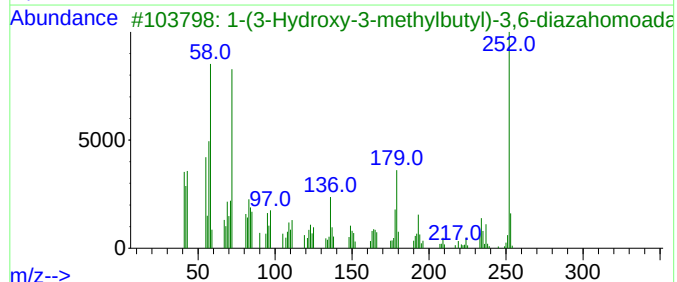
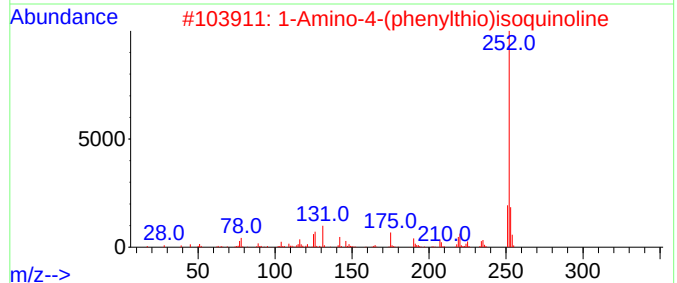
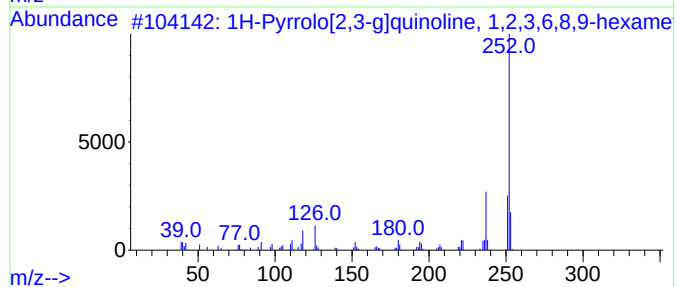
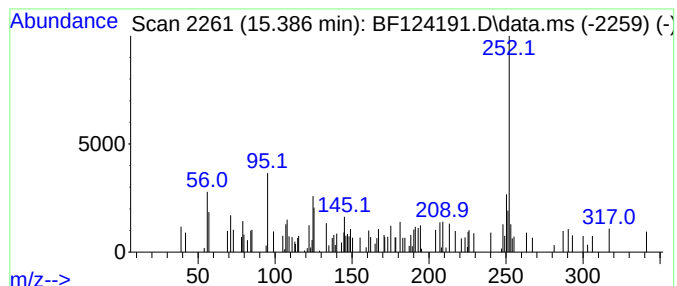
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown15.386 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.386	2.26 ng	25912	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Pyrrolo[2,3-g]quinoline, 1,2,...	252	C17H20N2	1000338-03-4	43
2			1-Amino-4-(phenylthio)isoquinoline	252	C15H12N2S	019653-19-1	38
3			1-(3-Hydroxy-3-methylbutyl)-3,6-...	252	C14H24N2O2	1000216-02-0	38
4			Thiazole, 2-amino-4-(4-biphenyl)-	252	C15H12N2S	002834-79-9	38
5			Rhodium, [(1,2,5,6-.eta.)-1,5-cy...	252	C11H17Rh	012176-45-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
Data File : BF124191.D
Acq On : 8 Jun 2021 21:17
Operator : JU/CG
Sample : M2629-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OK-02-060721

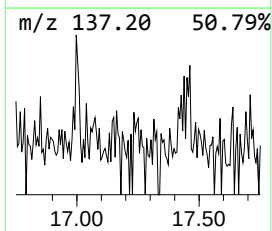
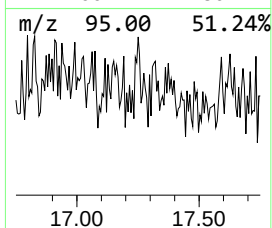
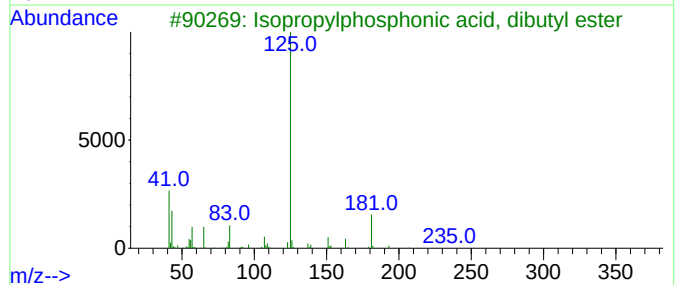
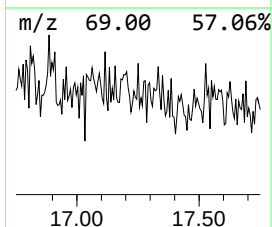
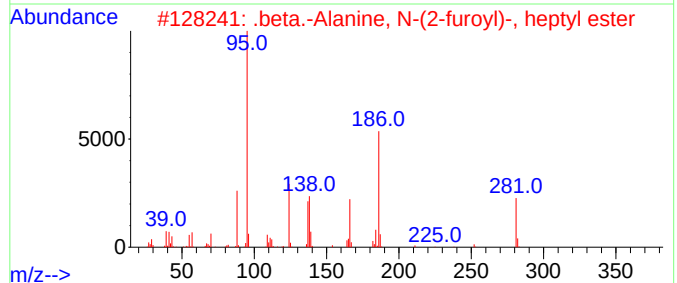
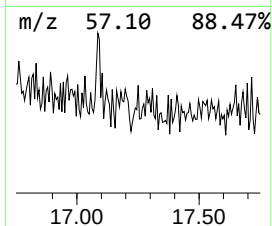
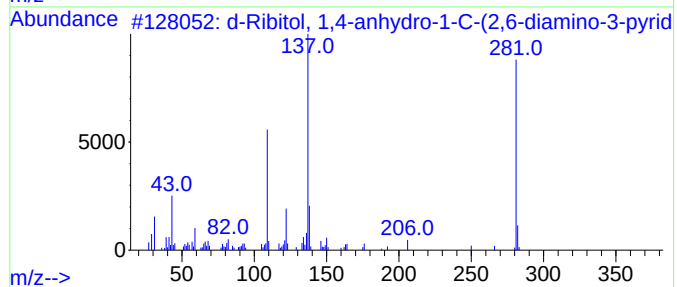
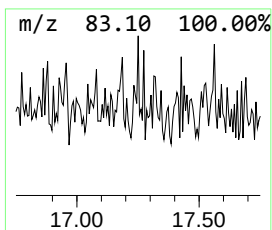
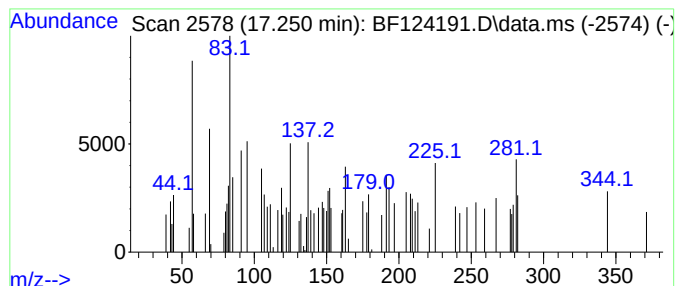
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown17.250 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.250	2.39 ng	27448	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			d-Ribitol, 1,4-anhydro-1-C-(2,6-...	281	C13H19N3O4	133635-38-8	10
2			.beta.-Alanine, N-(2-furoyl)-, h...	281	C15H23NO4	1000321-97-7	9
3			Isopropylphosphonic acid, dibuty...	236	C11H25O3P	000919-21-1	9
4			[2]Benzopyrano[4,3-b][1]benzopyr...	344	C19H20O6	014991-62-9	7
5			5-(7-Isopropyl-10-methyl-1,5-dit...	344	C18H32O2S2	1000189-29-2	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
Data File : BF124191.D
Acq On : 8 Jun 2021 21:17
Operator : JU/CG
Sample : M2629-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OK-02-060721

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.146	43.1	ng	566896	1	6.863	263030	20.0
unknown5.087	5.087	2.7	ng	36096	1	6.863	263030	20.0
9-Octadecenamid...	13.468	25.8	ng	417662	5	14.033	323942	20.0
Tetradecanamide	13.527	4.0	ng	64288	5	14.033	323942	20.0
13-Docosenamide...	14.798	40.1	ng	459600	6	15.515	229438	20.0
unknown15.386	15.386	2.3	ng	25912	6	15.515	229438	20.0
unknown17.080	17.080	2.2	ng	25372	6	15.515	229438	20.0
unknown17.250	17.250	2.4	ng	27448	6	15.515	229438	20.0