

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120324\
 Data File : BF140722.D
 Acq On : 03 Dec 2024 20:10
 Operator : RC/JU
 Sample : P5048-01
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-746-WC

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-BF112124.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140722.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	3	9	22	rVB	728683	1142681	68.61%	9.701%
2	2.258	22	28	38	rVB	24841	41724	2.51%	0.354%
3	5.093	505	510	520	rVB	55446	88009	5.28%	0.747%
4	5.504	574	580	605	rBV	1010754	1370964	82.31%	11.639%
5	6.510	745	751	769	rBV	1040841	1393863	83.69%	11.834%
6	6.869	807	812	819	rBV	306882	371073	22.28%	3.150%
7	7.434	902	908	917	rBV	677942	903016	54.22%	7.666%
8	7.687	944	951	962	rBV2	14594	32171	1.93%	0.273%
9	8.151	1025	1030	1042	rBV	348085	456365	27.40%	3.874%
10	9.222	1207	1212	1222	rBV	1341428	1665594	100.00%	14.141%
11	9.904	1323	1328	1343	rVB	370389	469564	28.19%	3.986%
12	10.616	1444	1449	1456	rBV	149071	193547	11.62%	1.643%
13	10.698	1458	1463	1477	rBV	622124	816451	49.02%	6.931%
14	11.398	1577	1582	1590	rBV	306707	429426	25.78%	3.646%
15	11.922	1663	1671	1682	rBV3	72990	160683	9.65%	1.364%
16	12.010	1683	1686	1695	rVB3	11737	28042	1.68%	0.238%
17	12.616	1784	1789	1793	rBV	55380	72779	4.37%	0.618%
18	12.845	1822	1828	1834	rBV	64812	102147	6.13%	0.867%
19	12.980	1846	1851	1860	rVB	905067	1159325	69.60%	9.842%
20	13.874	1999	2003	2015	rVB3	66727	124601	7.48%	1.058%
21	14.051	2028	2033	2045	rVB	276529	432544	25.97%	3.672%
22	15.557	2284	2289	2299	rVB	205759	324287	19.47%	2.753%

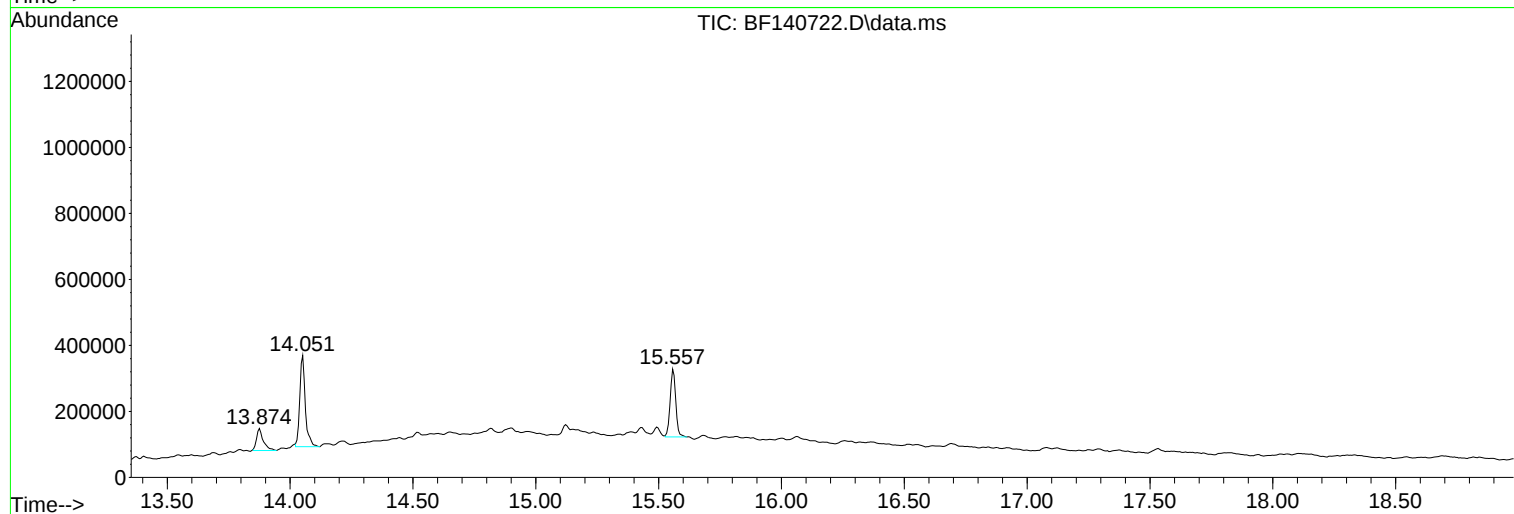
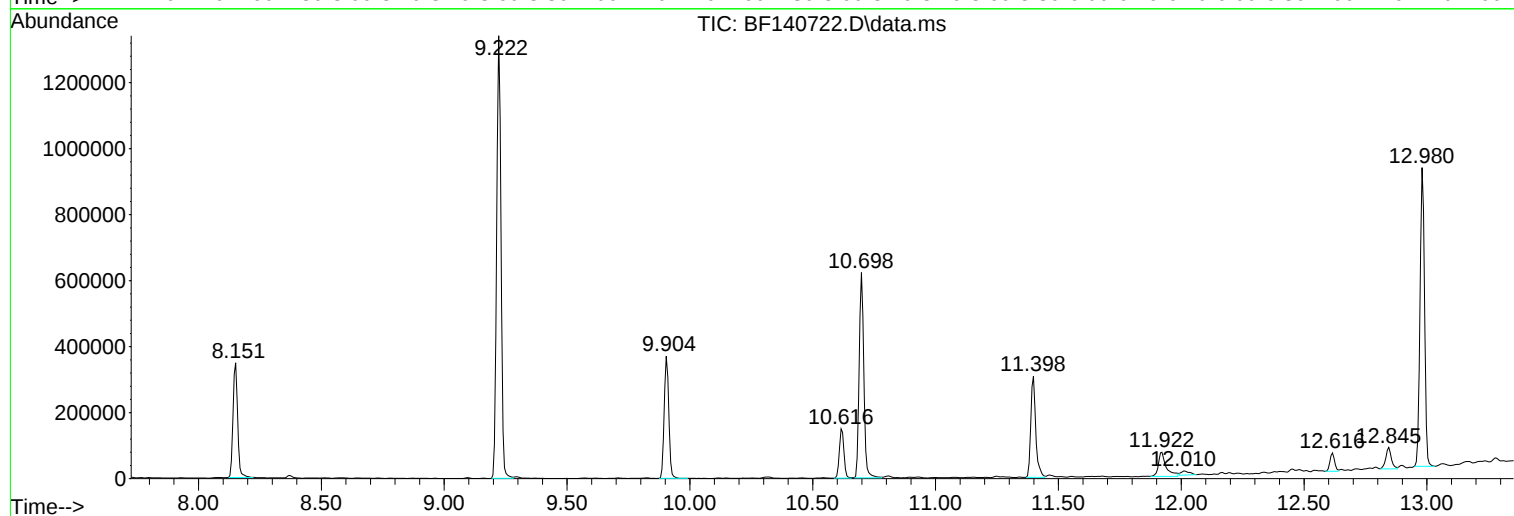
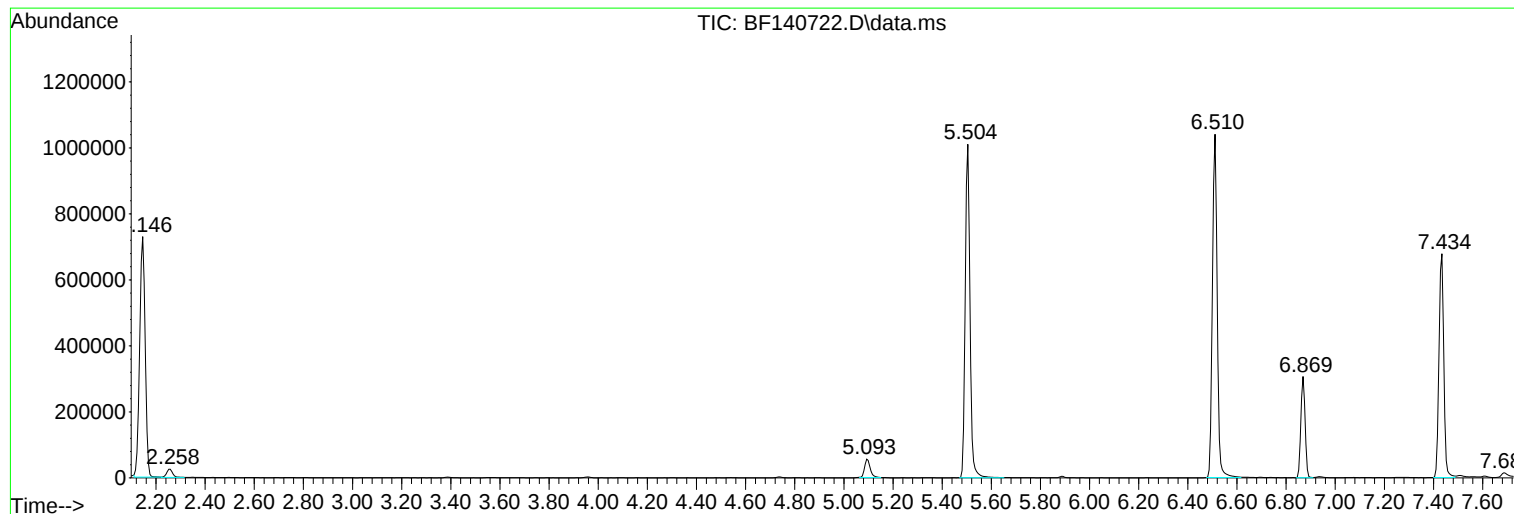
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120324\
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Instrument :
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ClientSampleId :
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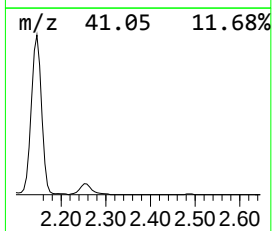
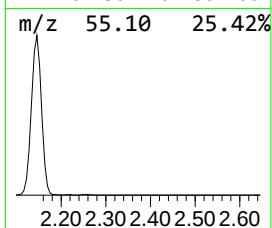
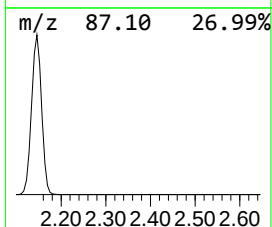
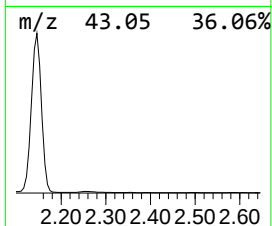
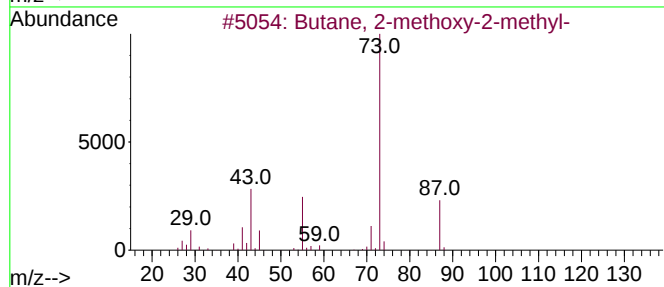
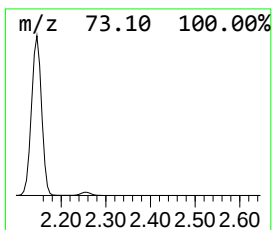
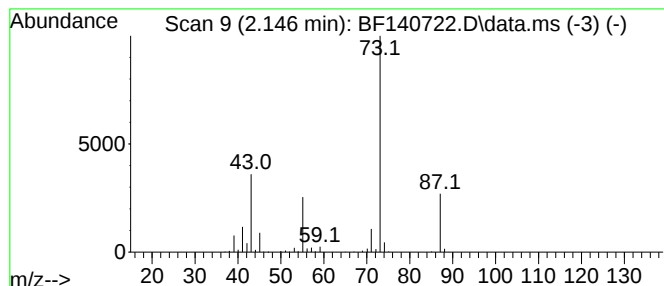
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	61.59 ng	1142680	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	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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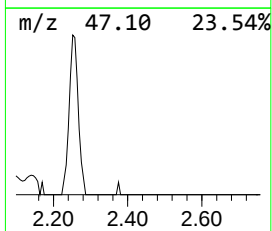
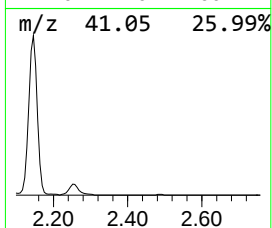
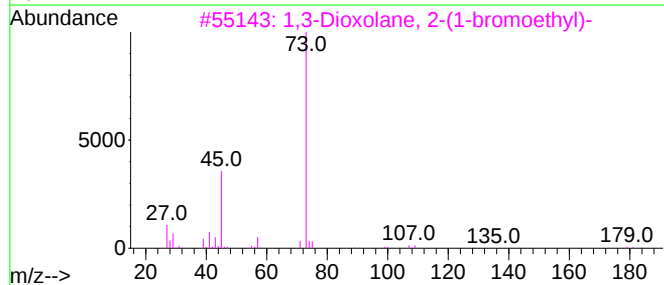
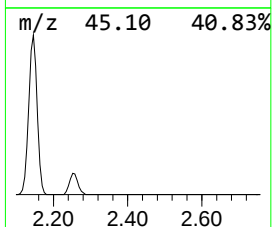
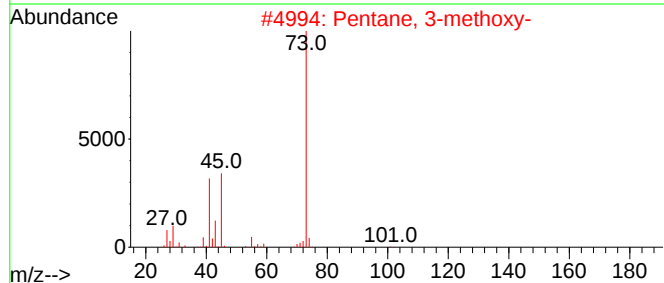
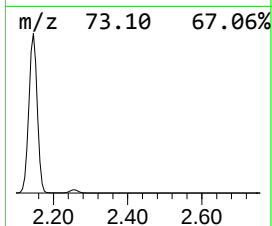
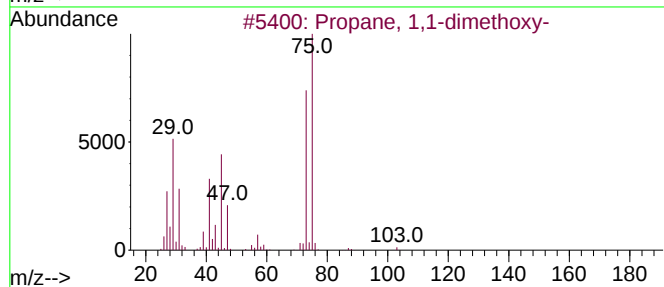
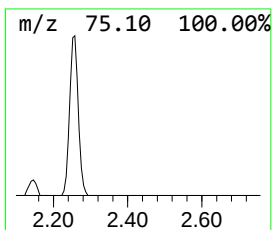
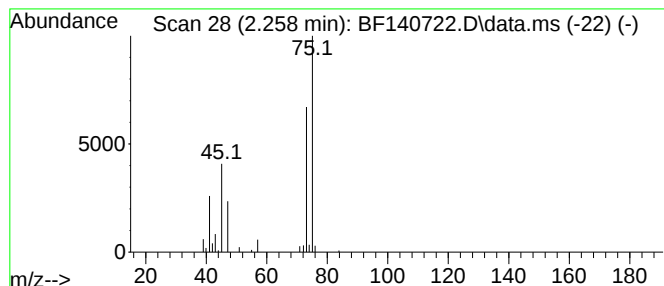
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.258	2.25 ng	41724	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
3			1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9
4			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	7
5			Glycine	75	C2H5NO2	000056-40-6	7



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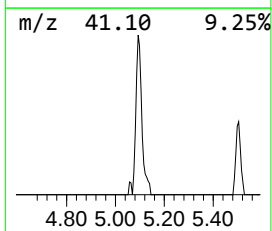
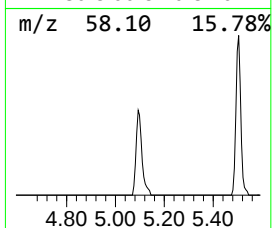
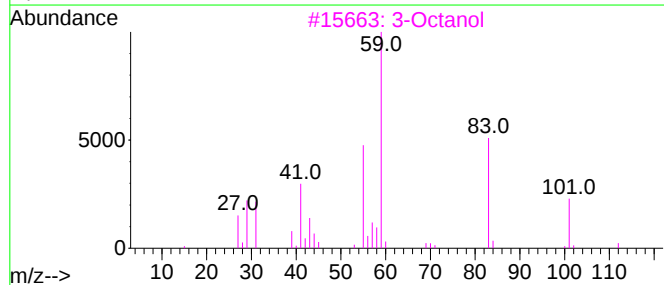
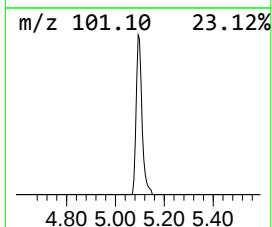
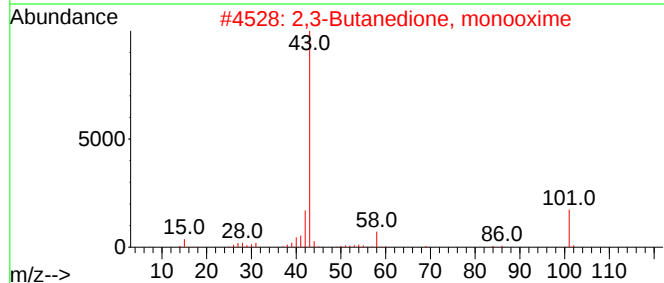
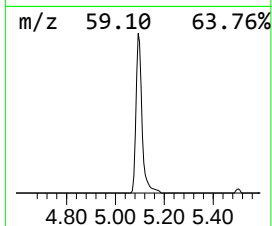
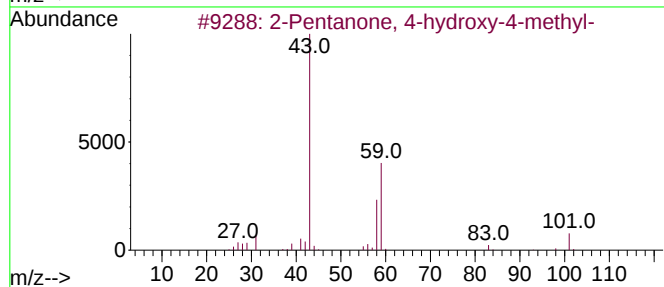
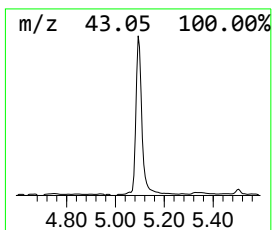
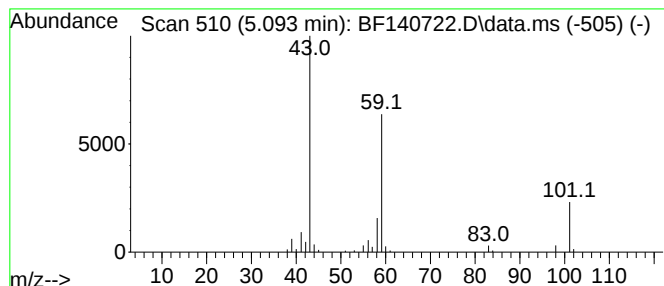
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	4.74 ng	88009	1,4-Dichlorobenzene-d4	6.869

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3		3-Octanol	130	C8H18O	000589-98-0	33
4		3-Hexanol	102	C6H14O	000623-37-0	33
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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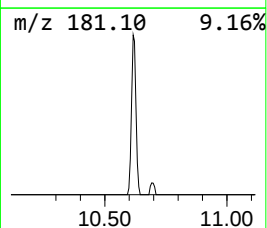
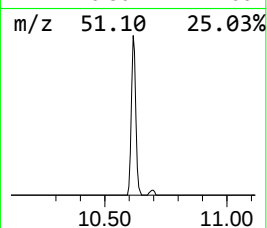
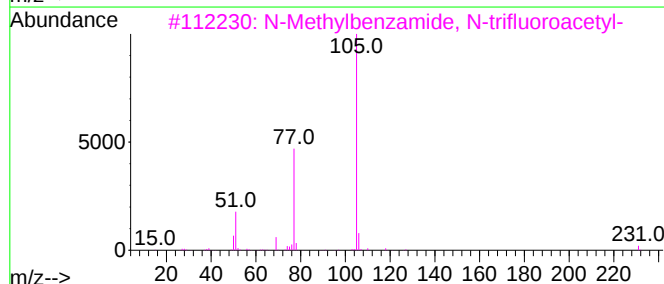
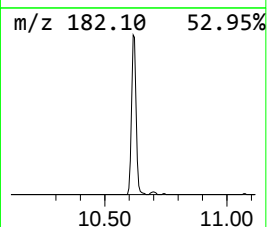
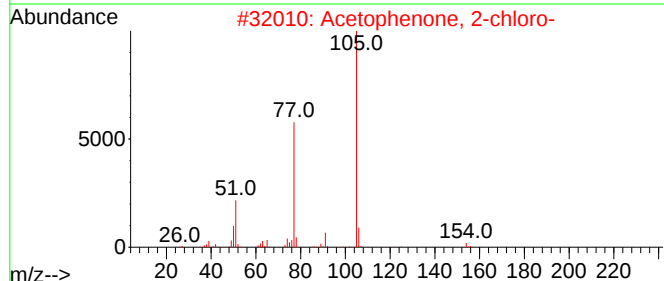
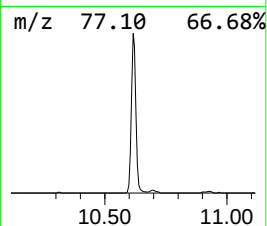
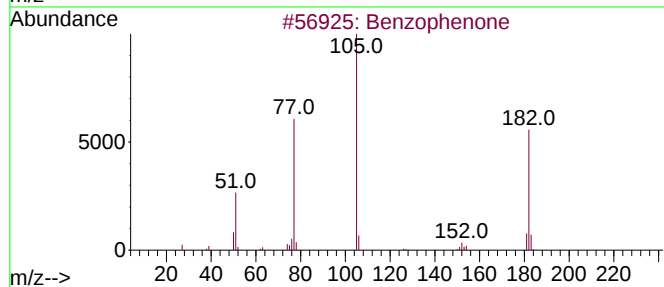
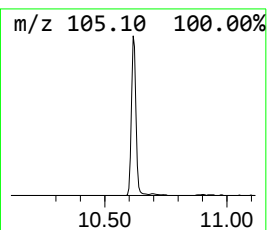
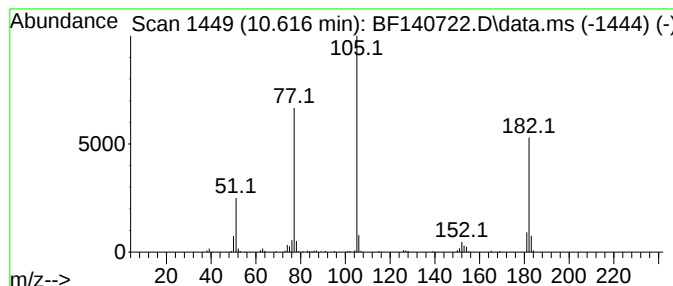
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	8.24 ng	193547	Acenaphthene-d10	9.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5			Ethanone, 2-bromo-1-phenyl-	198	C8H7BrO	000070-11-1	47



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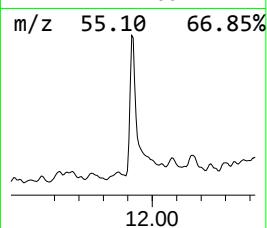
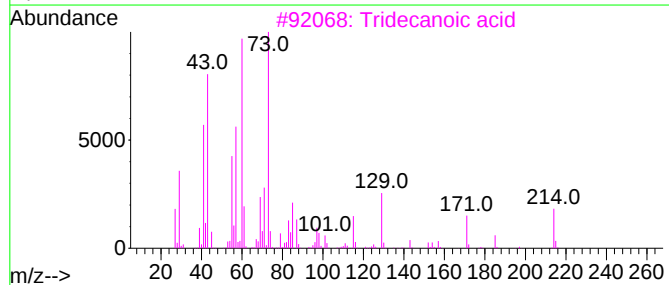
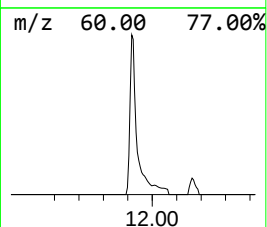
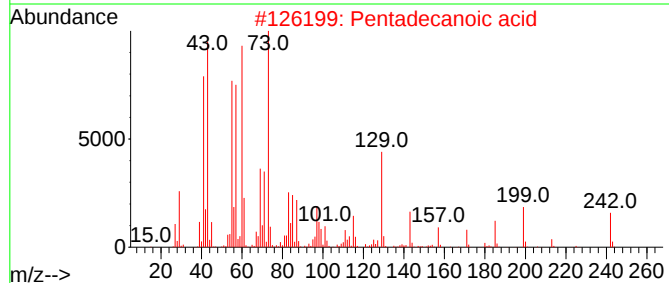
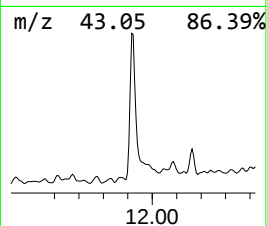
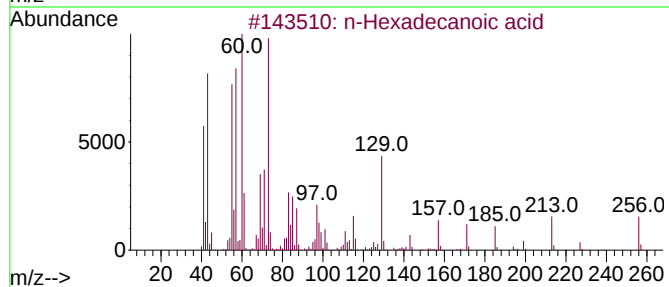
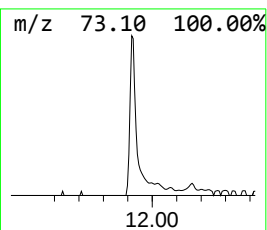
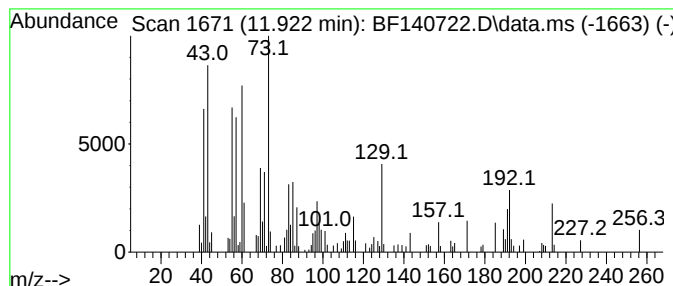
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TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	7.48 ng	160683	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3			Tridecanoic acid	214	C13H26O2	000638-53-9	70
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	53



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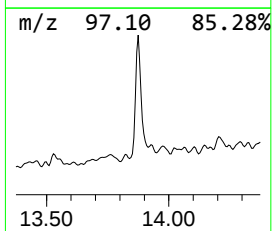
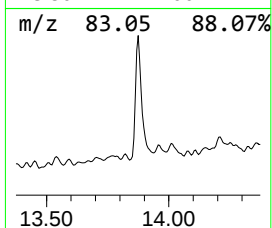
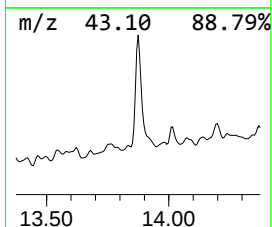
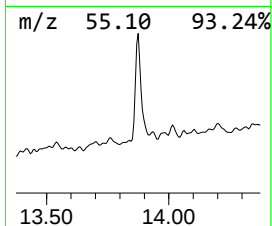
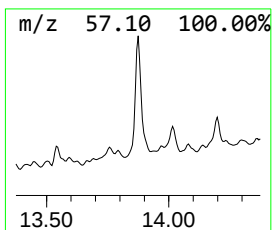
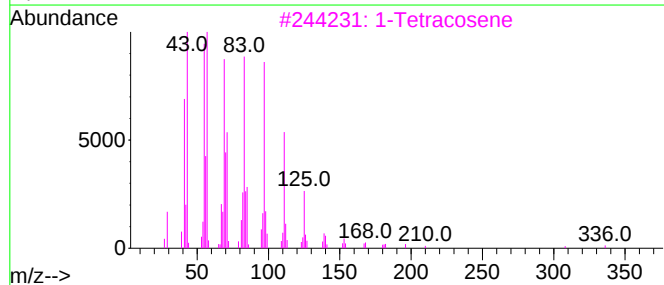
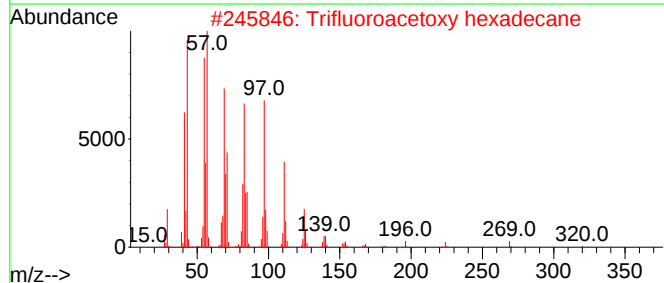
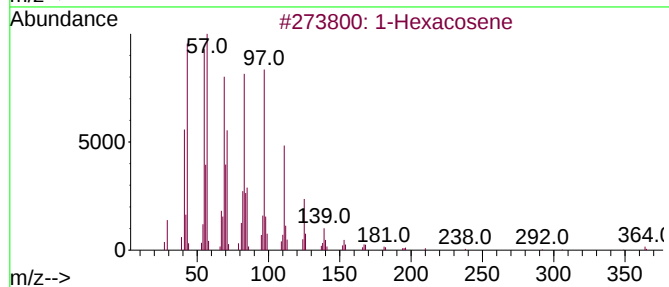
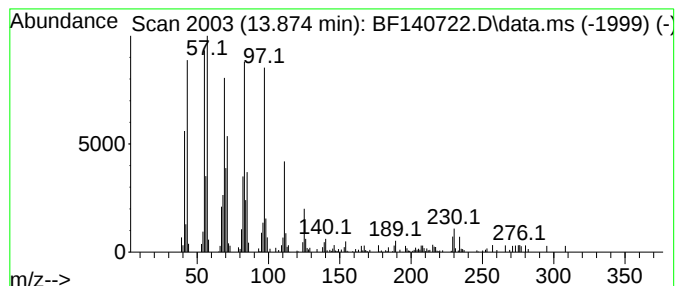
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Hexacosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	5.76 ng	124601	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexacosene	364	C26H52	018835-33-1	94
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3			1-Tetracosene	336	C24H48	010192-32-2	91
4			1-Heptacosanol	396	C27H56O	002004-39-9	91
5			1-Heneicosanol	312	C21H44O	015594-90-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120324\
Data File : BF140722.D
Acq On : 03 Dec 2024 20:10
Operator : RC/JU
Sample : P5048-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-746-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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...	2.146	61.6	ng	1142680	1	6.869	371073	20.0
Propane, 1,1-di...	2.258	2.3	ng	41724	1	6.869	371073	20.0
2-Pentanone, 4-...	5.093	4.7	ng	88009	1	6.869	371073	20.0
Benzophenone	10.616	8.2	ng	193547	3	9.904	469564	20.0
n-Hexadecanoic ...	11.922	7.5	ng	160683	4	11.398	429426	20.0
1-Hexacosene	13.874	5.8	ng	124601	5	14.051	432544	20.0