

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032125\
 Data File : BF142028.D
 Acq On : 21 Mar 2025 14:22
 Operator : RC/JU
 Sample : Q1619-07
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-2

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-BF031025.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142028.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	3	10	20	rBV	938464	1487250	46.16%	6.271%
2	5.093	500	510	517	rBV2	44265	83909	2.60%	0.354%
3	5.493	571	578	589	rBV	1966348	2693566	83.59%	11.358%
4	6.498	742	749	762	rBV	1985956	2847225	88.36%	12.005%
5	6.875	808	813	820	rBV	658137	817966	25.39%	3.449%
6	7.434	902	908	918	rBV	1245696	1652364	51.28%	6.967%
7	7.687	946	951	963	rBV	55528	79141	2.46%	0.334%
8	8.157	1025	1031	1048	rBV	789064	1113353	34.55%	4.695%
9	8.369	1062	1067	1078	rBV	30988	47001	1.46%	0.198%
10	9.228	1207	1213	1223	rBV	2587876	3222184	100.00%	13.587%
11	9.910	1323	1329	1343	rVB	970051	1243550	38.59%	5.243%
12	10.622	1445	1450	1457	rBV	258179	333315	10.34%	1.405%
13	10.698	1457	1463	1474	rBV	1535634	2088675	64.82%	8.807%
14	11.392	1577	1581	1591	rBV	852909	1154203	35.82%	4.867%
15	11.916	1666	1670	1679	rBV2	83749	150371	4.67%	0.634%
16	12.704	1799	1804	1822	rVB2	120479	259446	8.05%	1.094%
17	12.980	1845	1851	1860	rBV	2133737	2744598	85.18%	11.573%
18	13.874	1999	2003	2017	rVB	92294	184710	5.73%	0.779%
19	14.033	2025	2030	2038	rVB	495097	665738	20.66%	2.807%
20	14.886	2171	2175	2183	rVB	74235	106283	3.30%	0.448%
21	15.504	2275	2280	2294	rVB	426821	741200	23.00%	3.125%

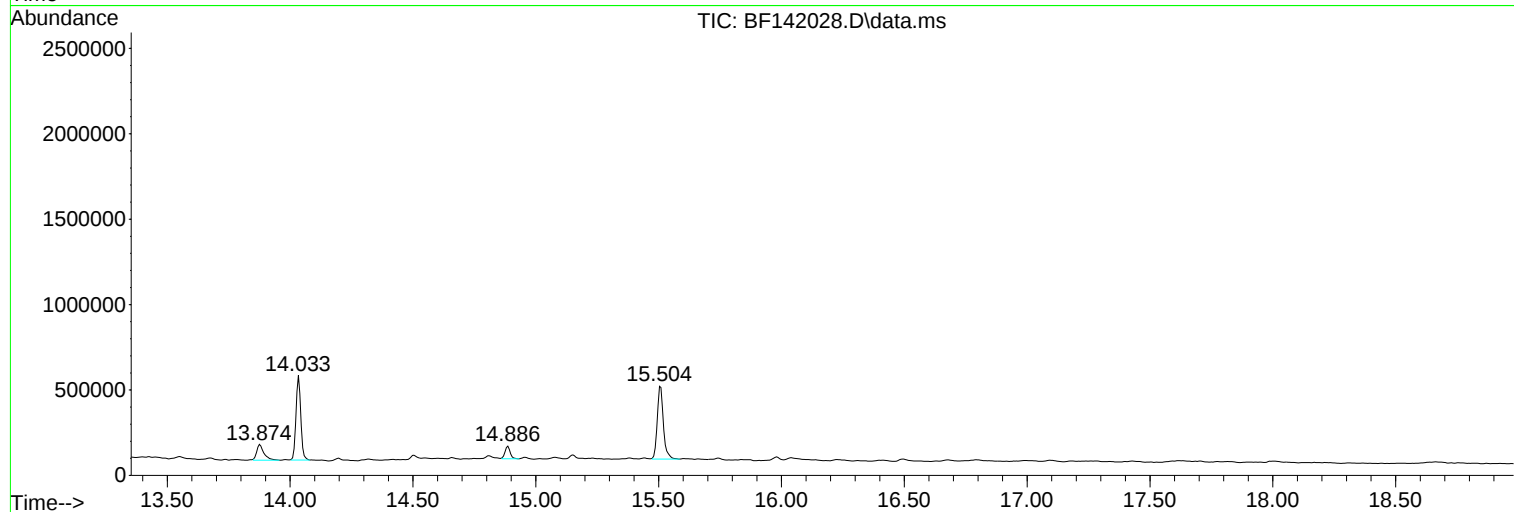
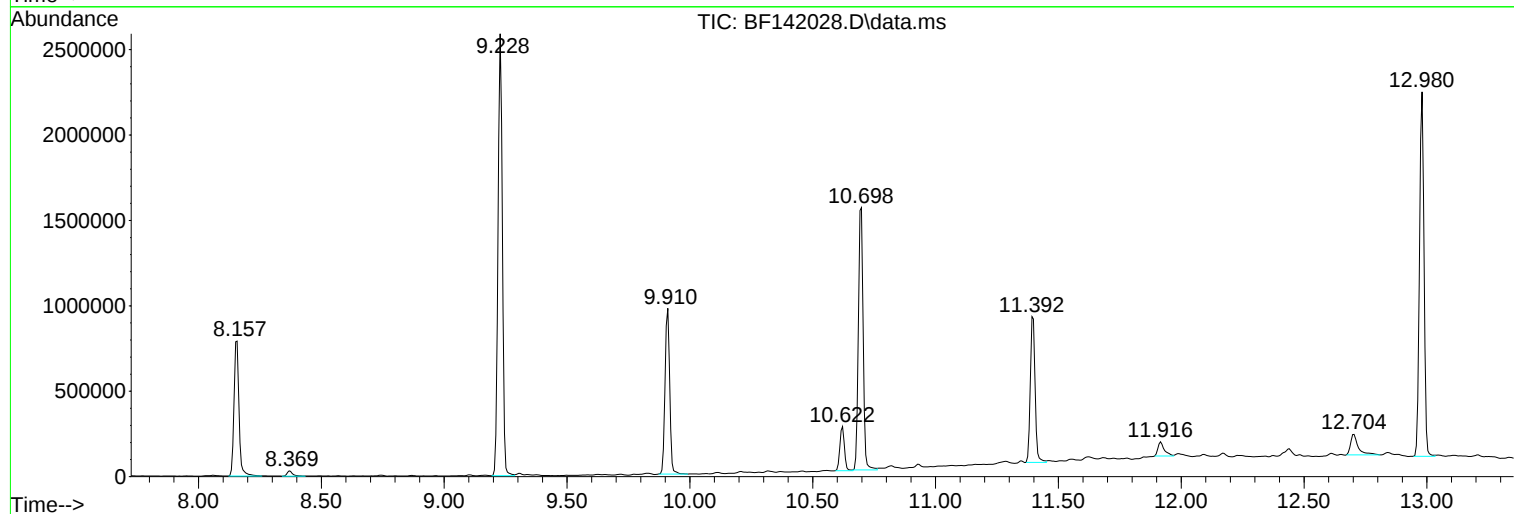
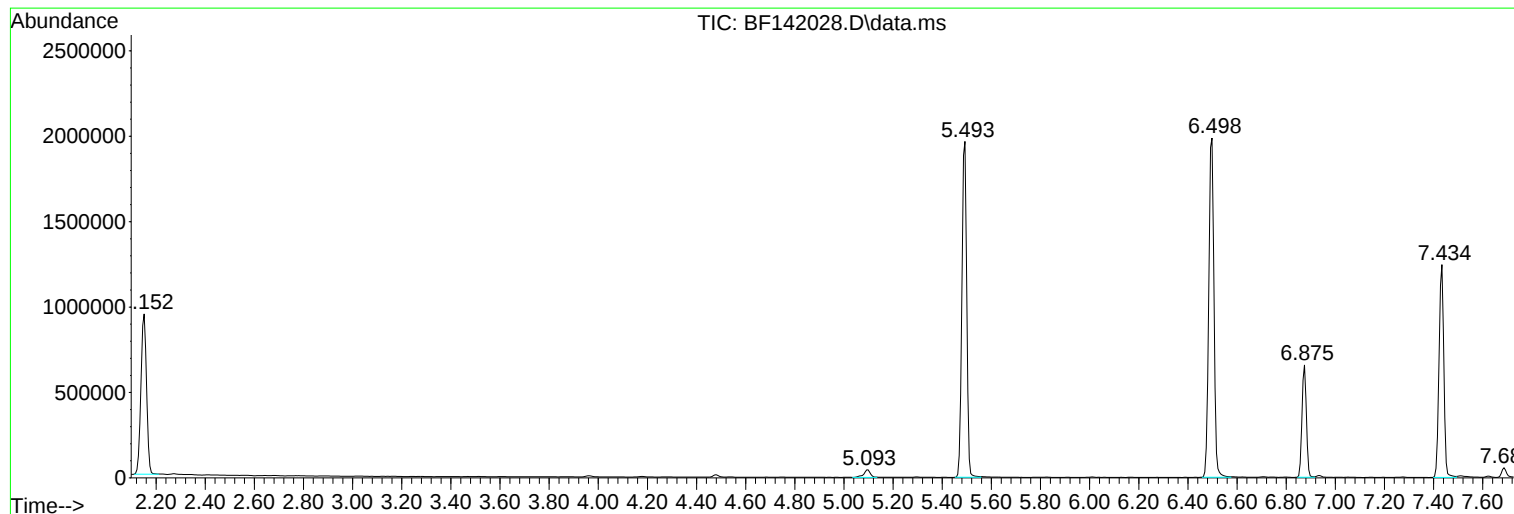
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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ClientSampleId :
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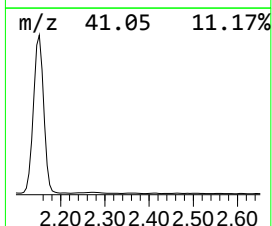
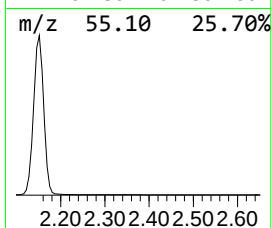
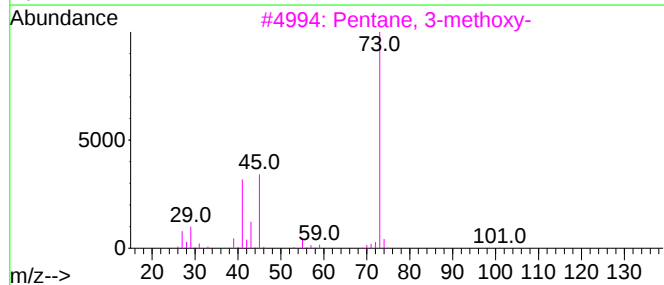
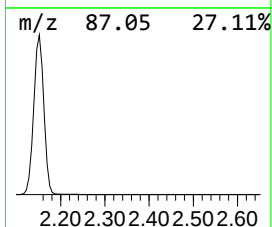
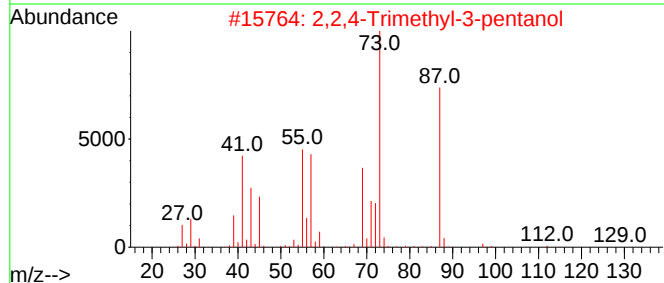
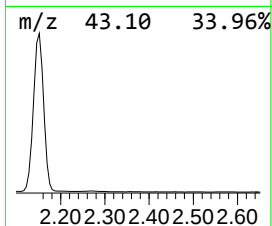
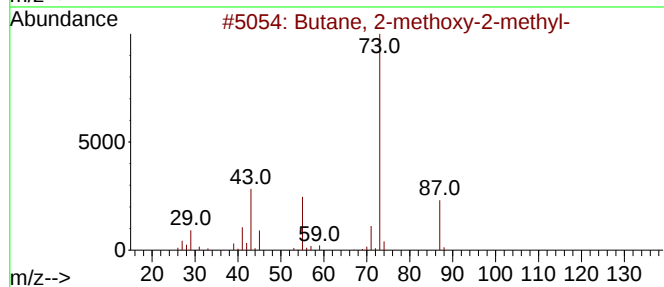
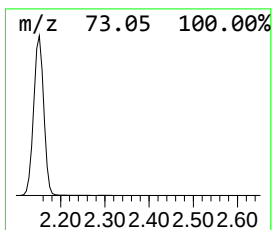
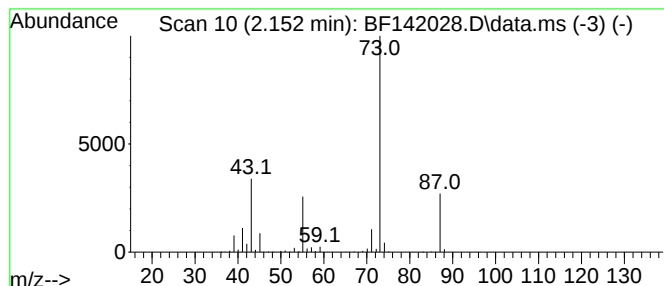
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	36.36 ng	1487250	1,4-Dichlorobenzene-d4	6.875

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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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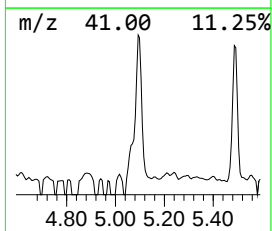
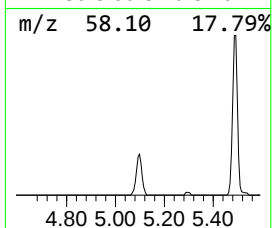
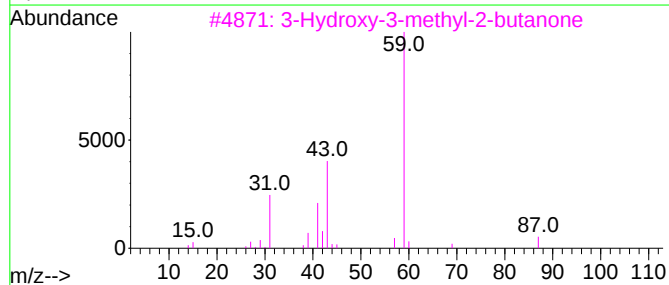
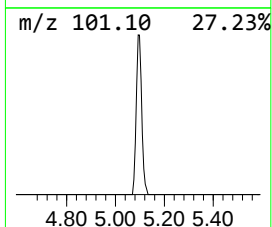
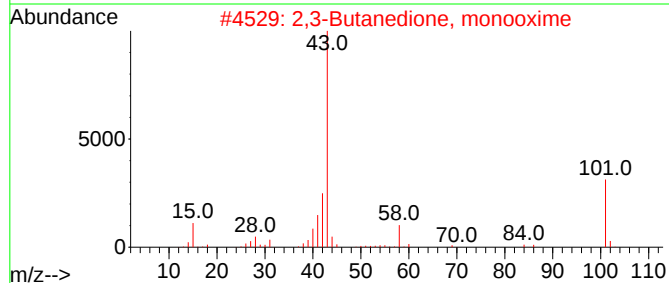
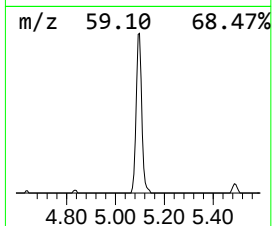
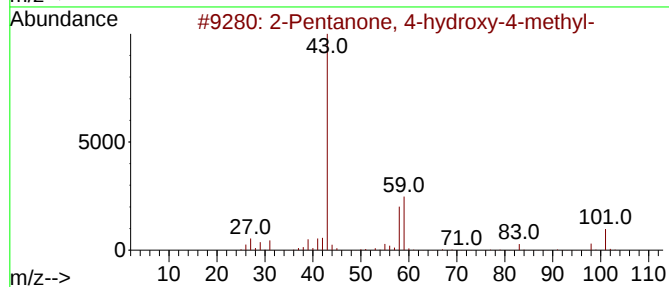
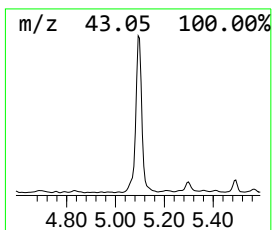
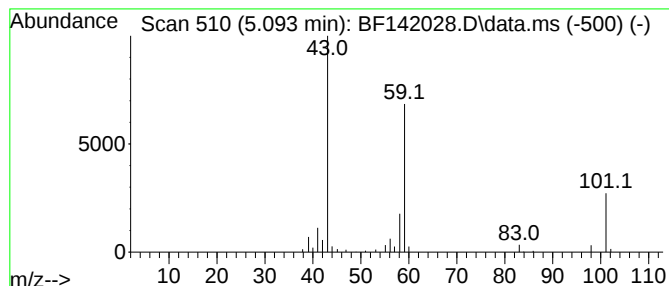
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	2.05 ng	83909	1,4-Dichlorobenzene-d4	6.875

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	16
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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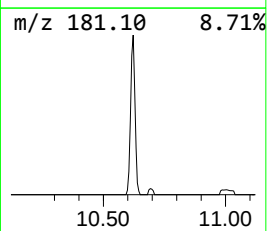
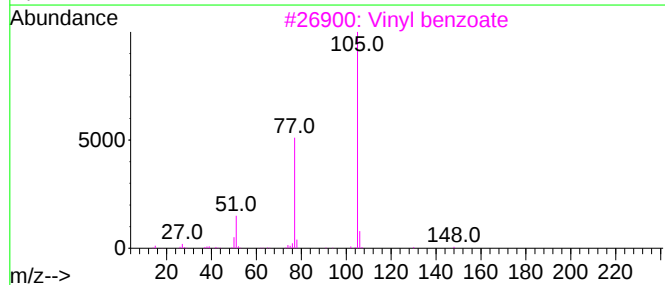
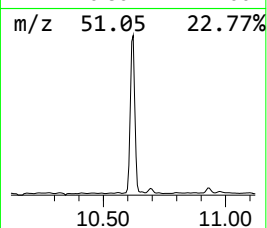
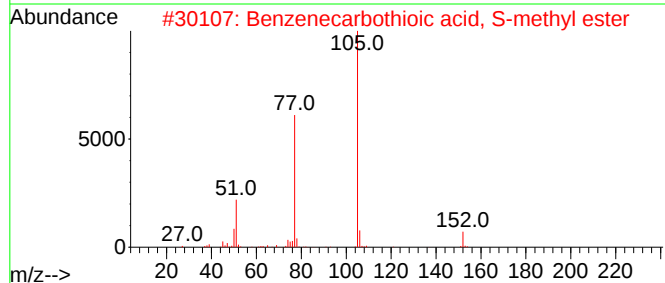
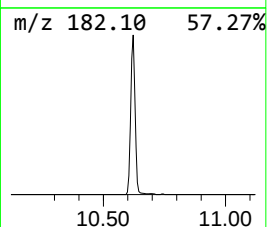
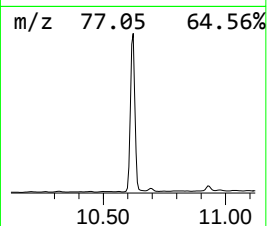
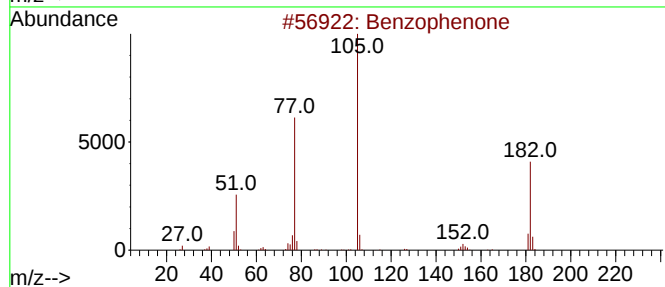
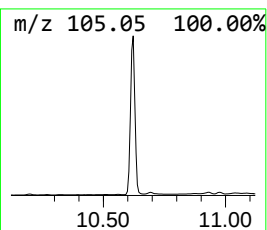
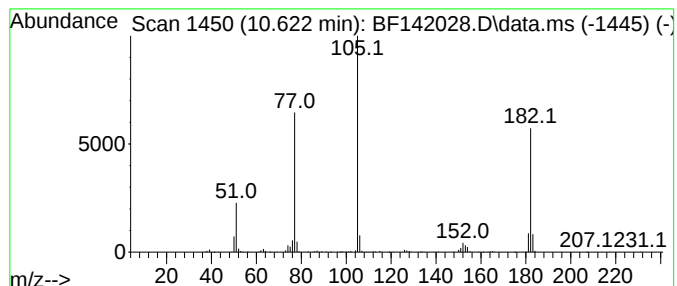
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	5.36 ng	333315	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
3			Vinyl benzoate	148	C9H8O2	000769-78-8	49
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
5			Benzenecarbothioic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47



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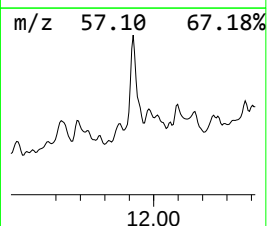
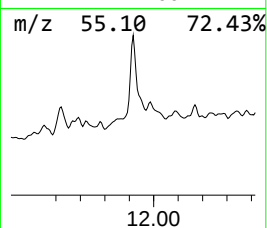
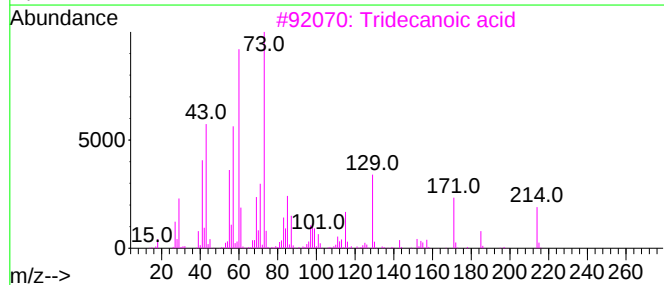
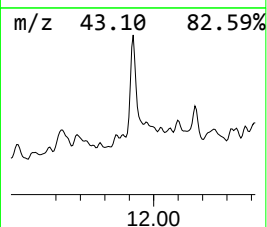
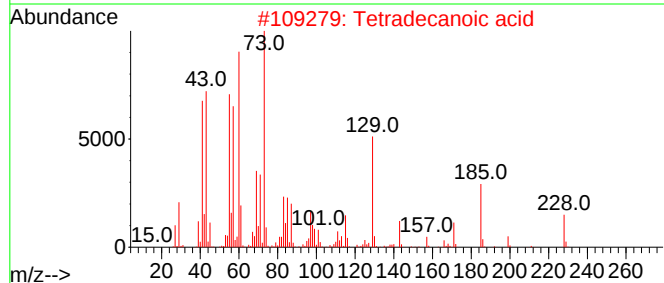
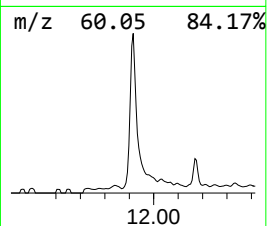
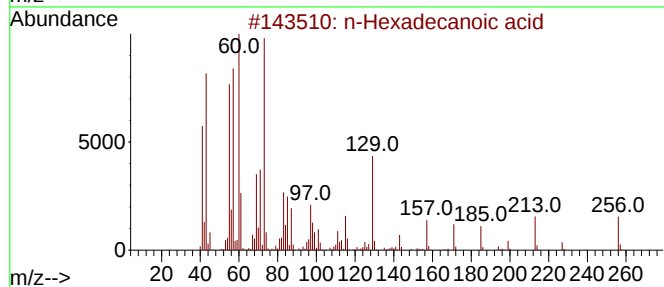
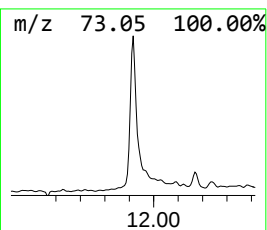
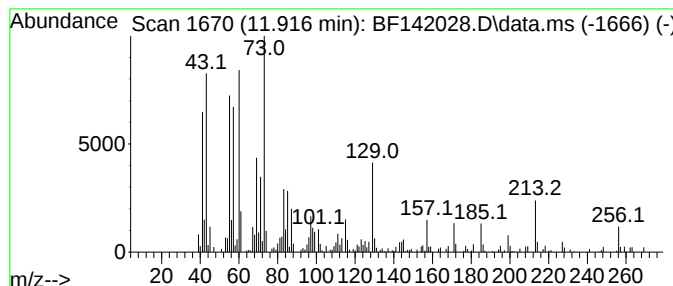
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	2.61 ng	150371	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			n-Decanoic acid	172	C10H20O2	000334-48-5	86
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	81



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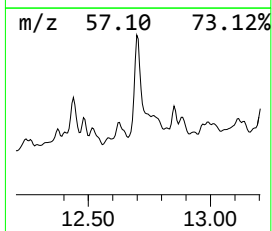
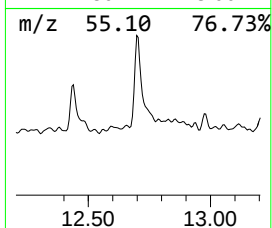
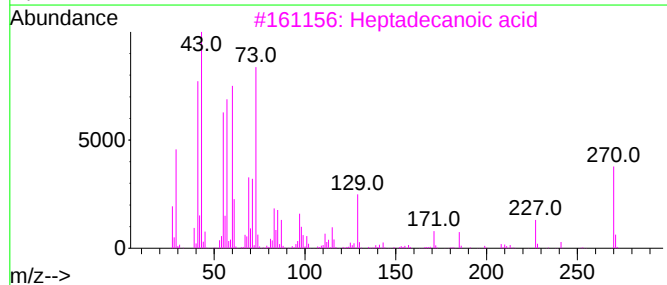
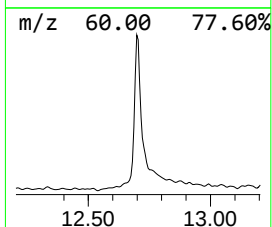
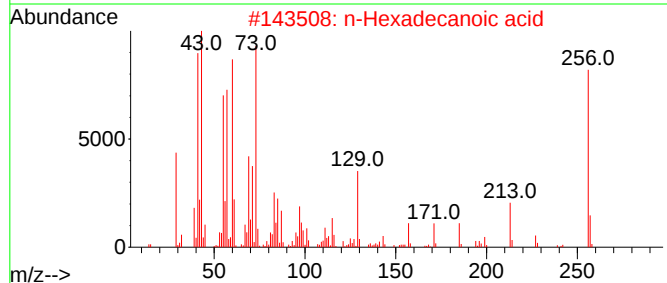
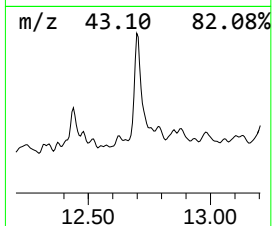
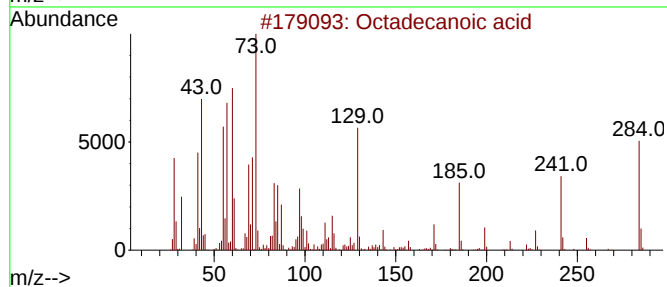
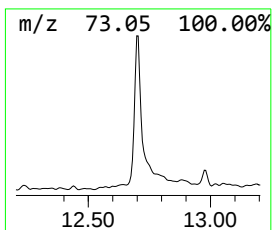
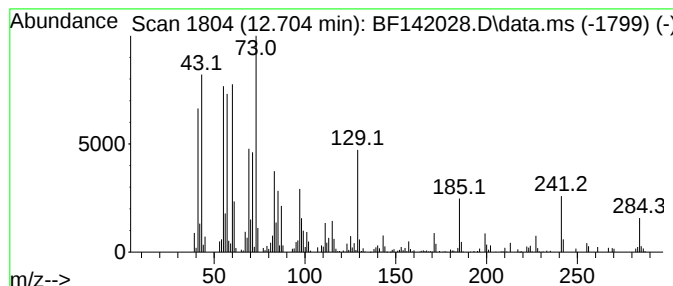
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	4.50 ng	259446	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Heptadecanoic acid	270	C17H34O2	000506-12-7	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	81



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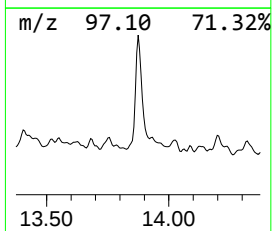
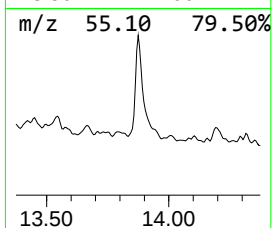
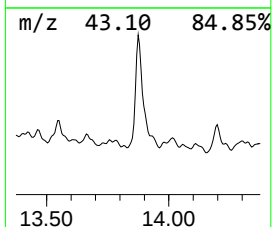
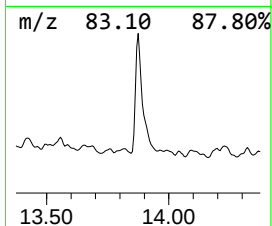
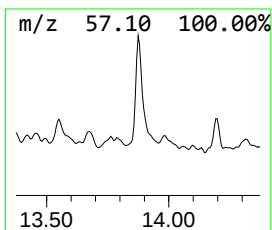
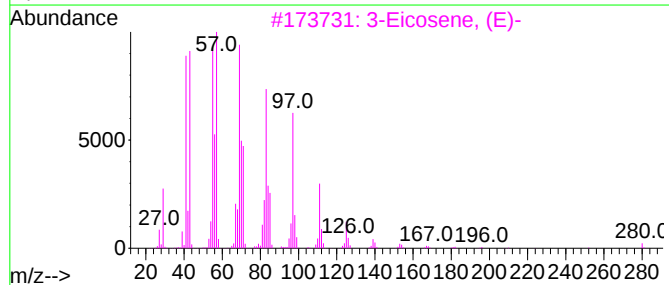
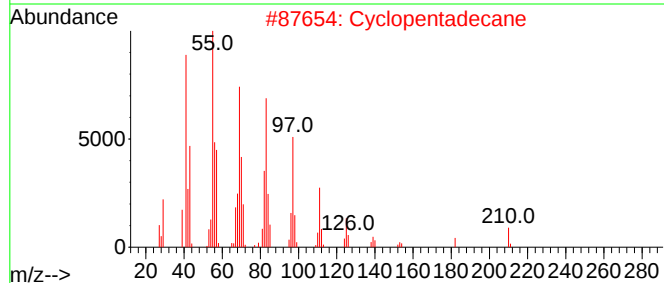
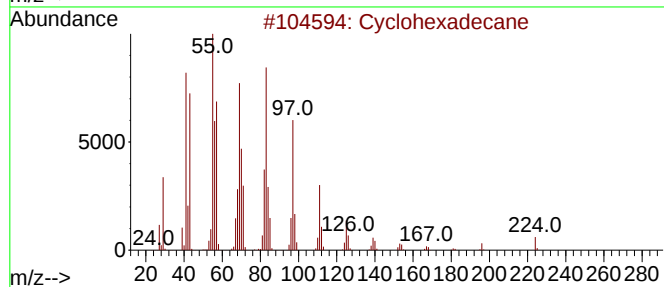
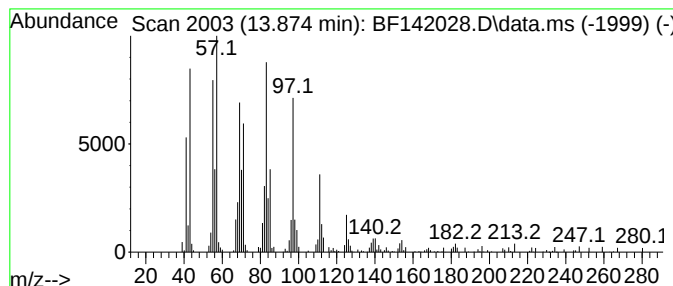
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclohexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	5.55 ng	184710	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	99
2			Cyclopentadecane	210	C15H30	000295-48-7	98
3			3-Eicosene, (E)-	280	C20H40	074685-33-9	97
4			5-Octadecene, (E)-	252	C18H36	007206-21-5	94
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032125\
Data File : BF142028.D
Acq On : 21 Mar 2025 14:22
Operator : RC/JU
Sample : Q1619-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

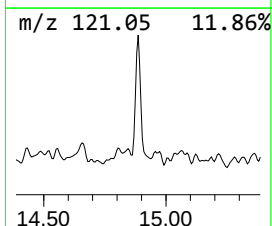
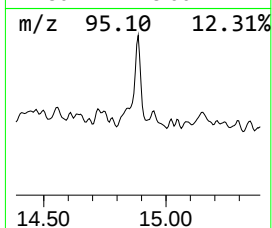
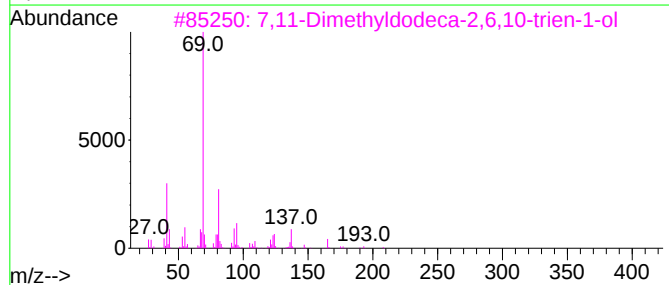
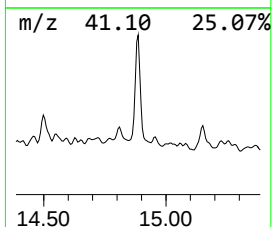
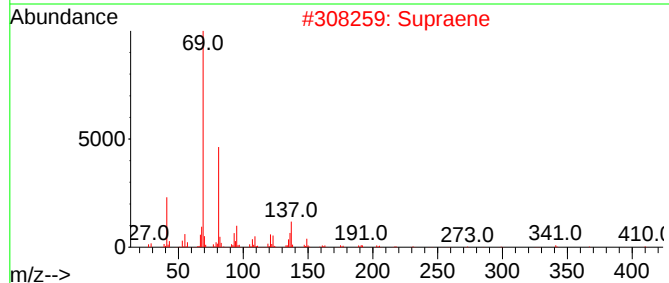
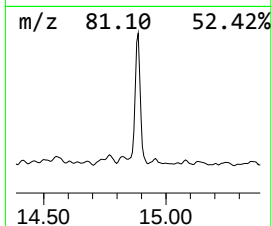
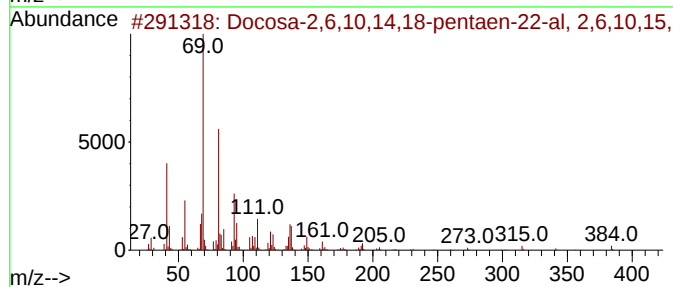
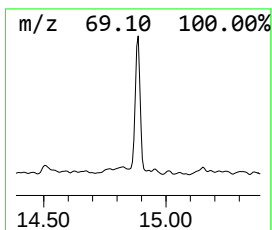
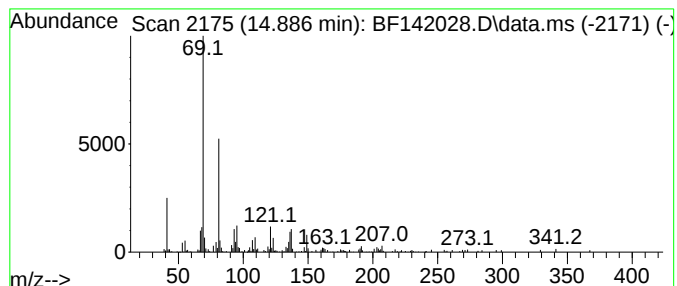
Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Docosa-2,6,10,14,18-pentaen... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.886	2.87 ng	106283	Perylene-d12	15.504	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
2	Supraene	410	C30H50	007683-64-9	83
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	74
4	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	72
5	4-Oxo-.beta.-damascone	206	C13H18O2	053398-08-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032125\
Data File : BF142028.D
Acq On : 21 Mar 2025 14:22
Operator : RC/JU
Sample : Q1619-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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...	2.152	36.4	ng	1487250	1	6.875	817966	20.0
2-Pentanone, 4-...	5.093	2.0	ng	83909	1	6.875	817966	20.0
Benzophenone	10.622	5.4	ng	333315	3	9.910	1243550	20.0
n-Hexadecanoic ...	11.916	2.6	ng	150371	4	11.392	1154200	20.0
Octadecanoic acid	12.704	4.5	ng	259446	4	11.392	1154200	20.0
Cyclohexadecane	13.874	5.5	ng	184710	5	14.033	665738	20.0
Docos-2,6,10,1...	14.886	2.9	ng	106283	6	15.504	741200	20.0