

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
 Data File : BF131595.D
 Acq On : 12 Dec 2022 16:31
 Operator : CG\JU
 Sample : N5964-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SU-518-COMP-01

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-BF120822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131595.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	8	16	23	rVB	464700	585779	35.53%	4.845%
2	2.287	30	34	41	rBV2	21642	26210	1.59%	0.217%
3	5.104	509	513	523	rVB	179590	223429	13.55%	1.848%
4	5.510	578	582	585	rBV	1480253	1428836	86.67%	11.819%
5	6.522	749	754	757	rBV	1424085	1485226	90.09%	12.285%
6	6.893	813	817	820	rBV	455828	378984	22.99%	3.135%
7	7.457	908	913	916	rBV	1046978	927274	56.25%	7.670%
8	8.181	1032	1036	1039	rBV	549343	476717	28.92%	3.943%
9	9.263	1214	1220	1223	rBV	1952067	1648589	100.00%	13.637%
10	9.945	1331	1336	1340	rVB	690033	562685	34.13%	4.654%
11	10.739	1467	1471	1474	rBV	1402215	1177396	71.42%	9.739%
12	11.439	1586	1590	1594	rBV	656168	590374	35.81%	4.883%
13	11.510	1598	1602	1605	rVB	22969	18839	1.14%	0.156%
14	11.969	1677	1680	1683	rBV	38963	33556	2.04%	0.278%
15	12.539	1770	1777	1785	rBV4	18059	23635	1.43%	0.196%
16	13.039	1857	1862	1865	rBV	1831321	1496628	90.78%	12.380%
17	13.604	1955	1958	1961	rBV	29658	26158	1.59%	0.216%
18	13.939	2010	2015	2018	rBV	40500	37820	2.29%	0.313%
19	13.998	2018	2025	2026	rBV3	38010	63914	3.88%	0.529%
20	14.098	2038	2042	2046	rVB	418934	358748	21.76%	2.967%
21	14.192	2053	2058	2063	rVB	57069	56809	3.45%	0.470%
22	14.257	2065	2069	2072	rBV	47386	40536	2.46%	0.335%
23	14.563	2118	2121	2125	rBV	43462	36144	2.19%	0.299%
24	14.880	2170	2175	2179	rBV	27146	31388	1.90%	0.260%
25	15.239	2232	2236	2241	rVB2	18321	21155	1.28%	0.175%
26	15.610	2294	2299	2311	rVB	246440	332552	20.17%	2.751%

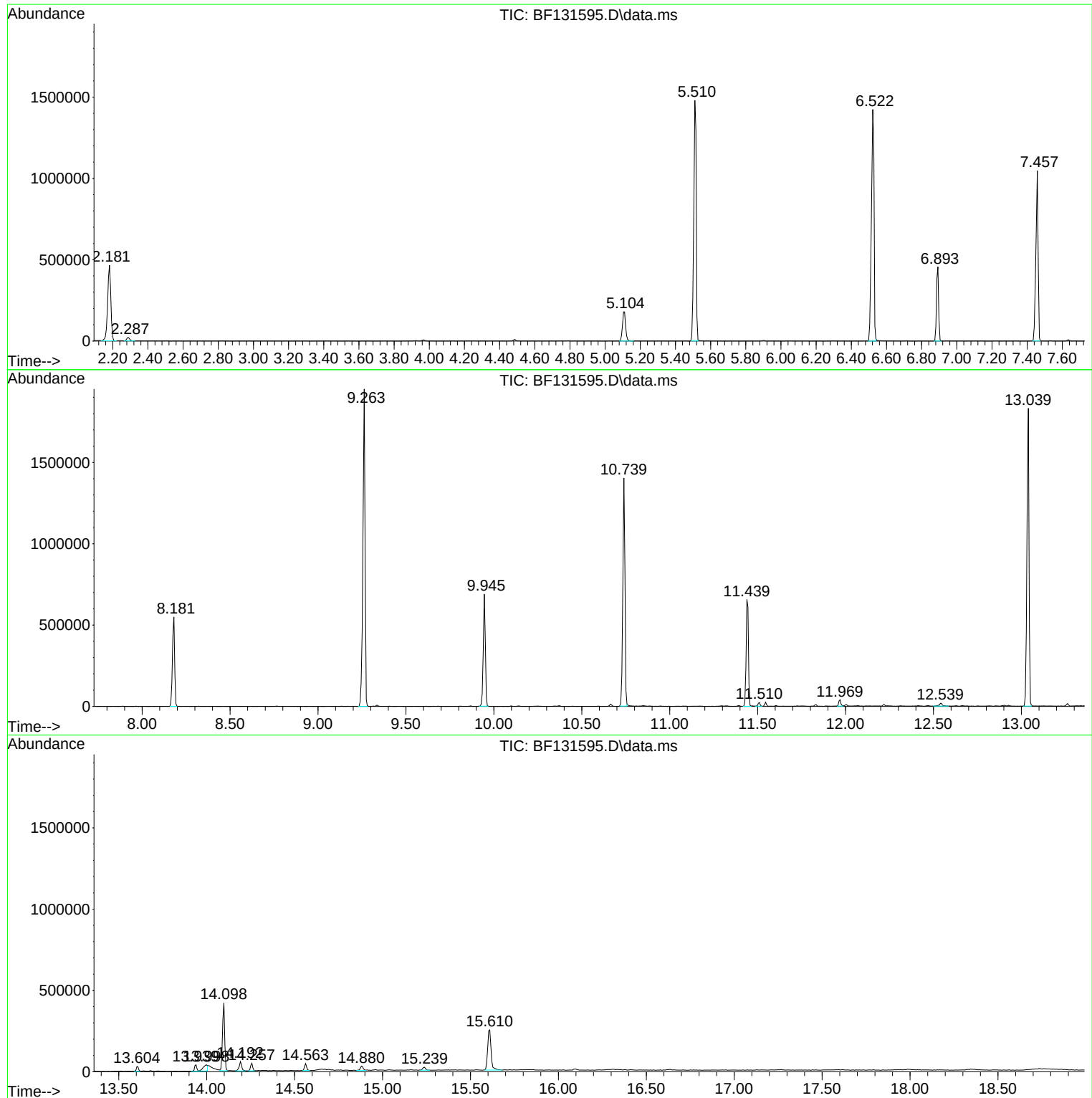
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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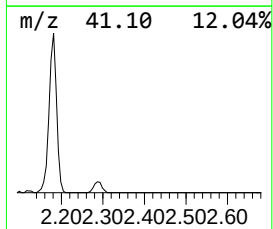
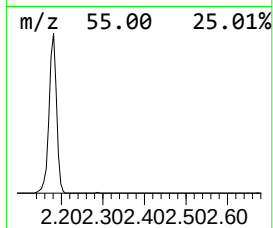
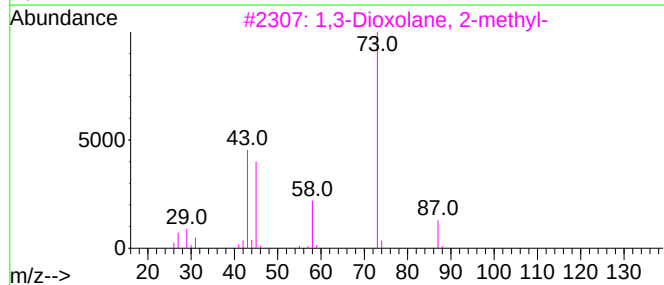
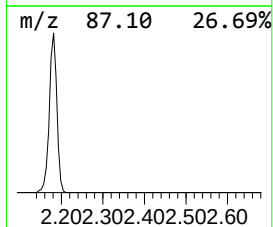
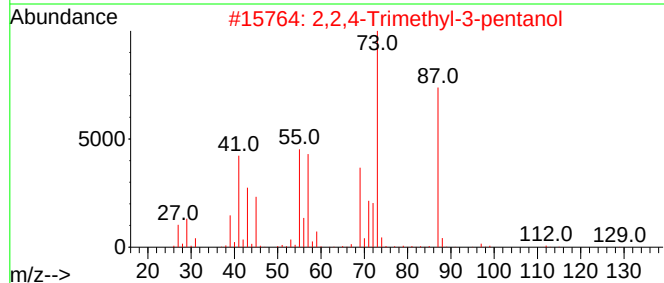
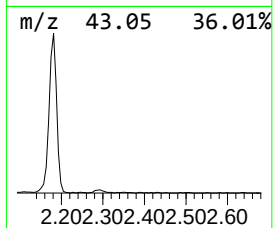
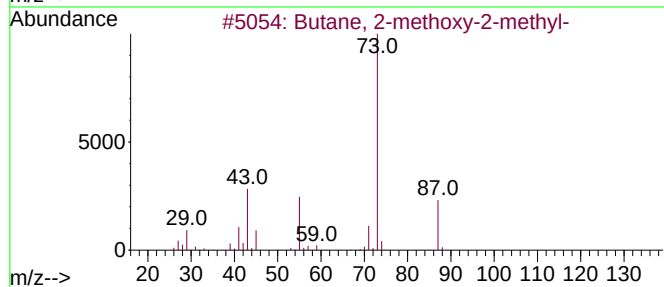
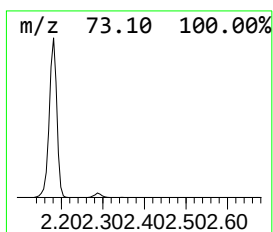
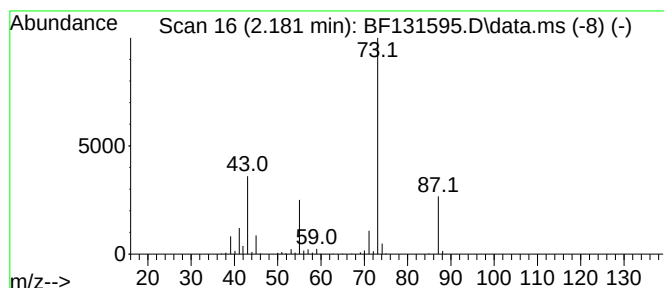
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.181	30.91 ng	585779	1,4-Dichlorobenzene-d4	6.893

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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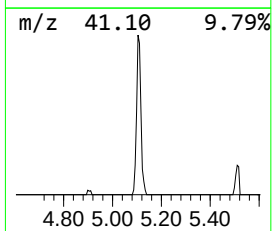
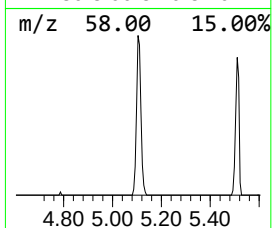
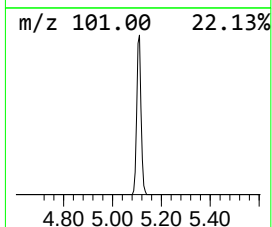
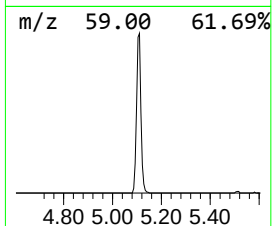
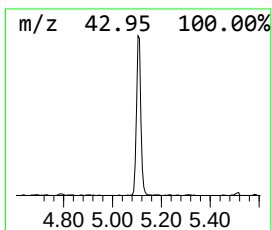
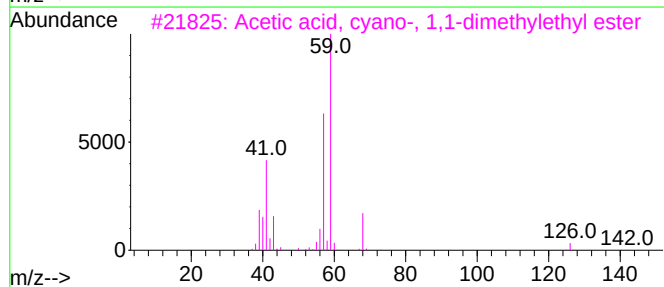
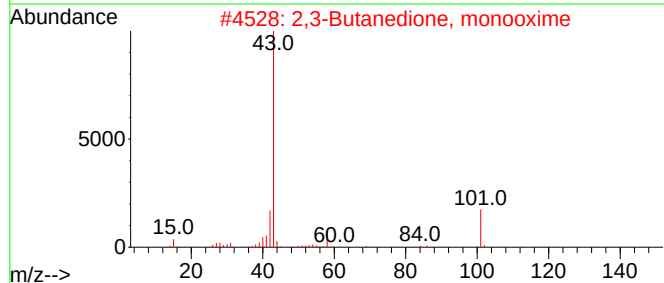
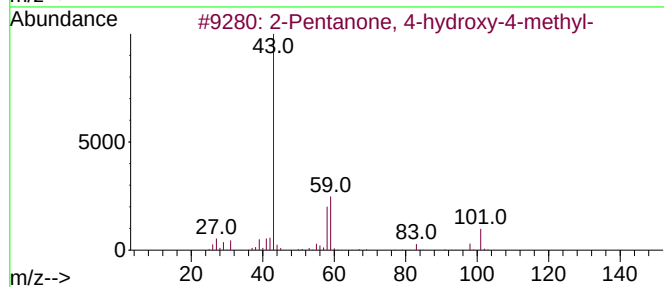
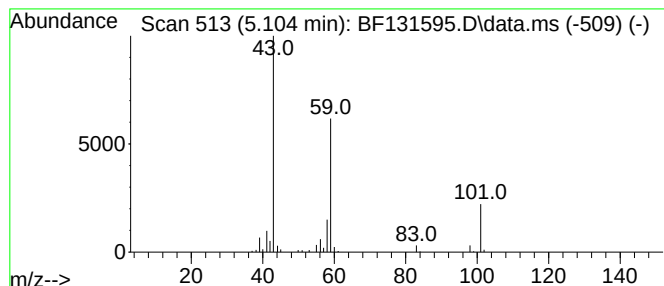
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	11.79 ng	223429	1,4-Dichlorobenzene-d4	6.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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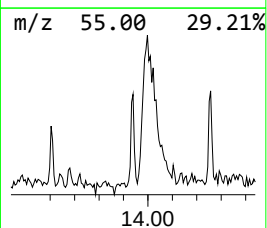
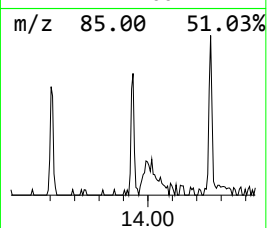
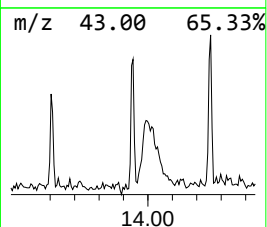
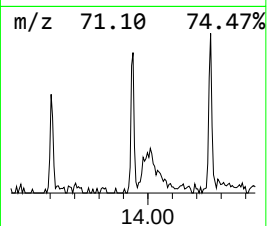
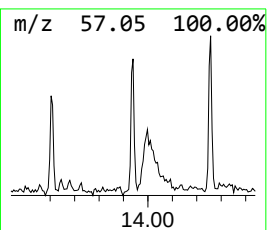
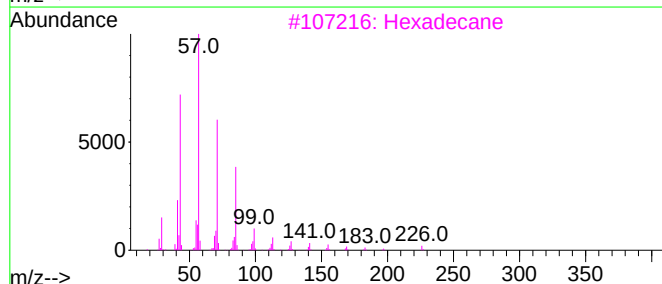
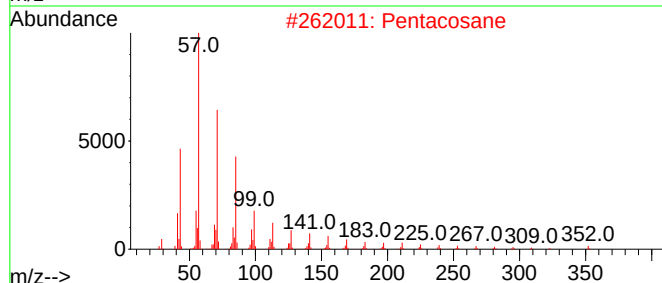
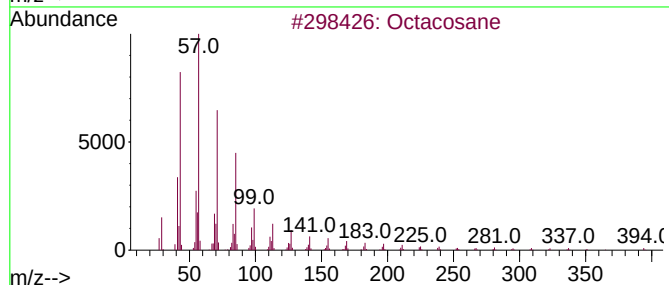
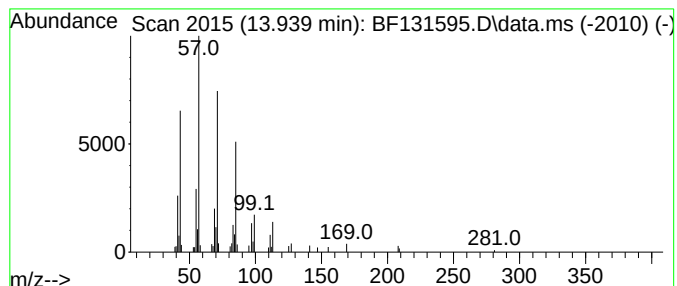
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	2.11 ng	37820	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Pentacosane	352	C25H52	000629-99-2	86
3			Hexadecane	226	C16H34	000544-76-3	59
4			Sulfurous acid, pentadecyl penty...	362	C20H42O3S	1000309-14-8	58
5			Sulfurous acid, isohexyl pentyl ...	236	C11H24O3S	1000309-14-0	58



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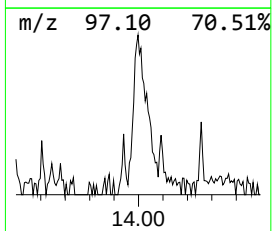
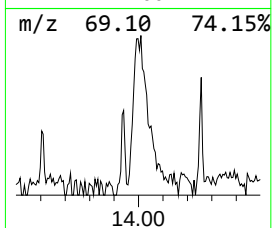
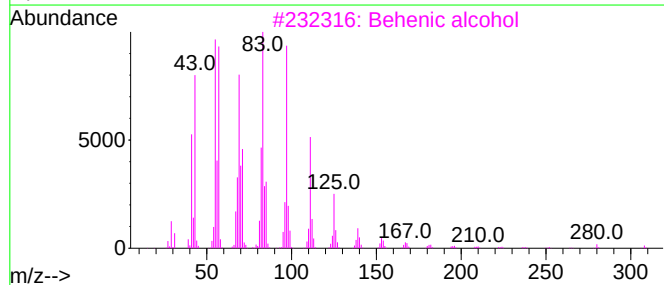
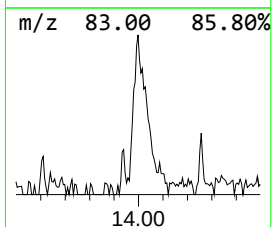
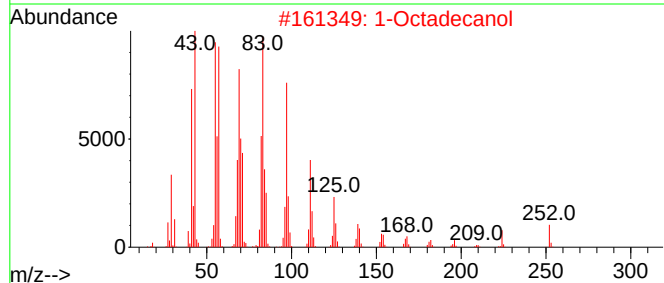
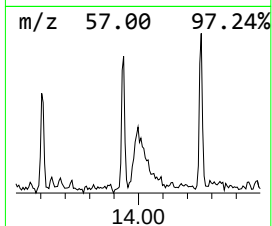
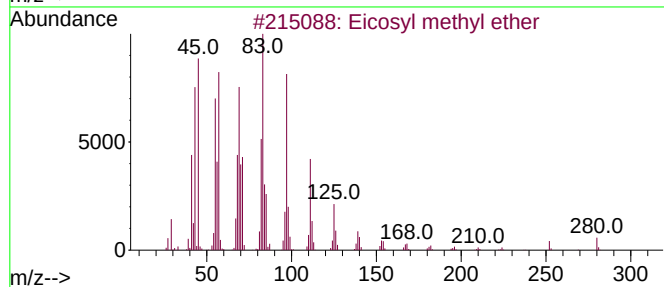
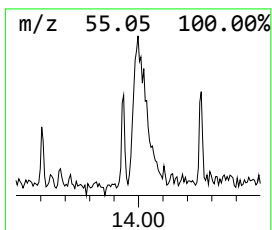
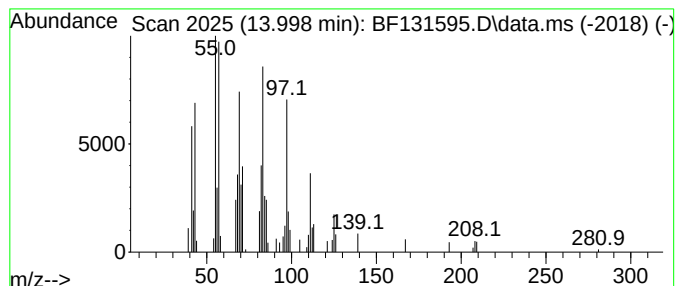
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Eicosyl methyl ether Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	3.56 ng	63914	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosyl methyl ether	312	C21H44O	1000406-29-4	94
2			1-Octadecanol	270	C18H38O	000112-92-5	91
3			Behenic alcohol	326	C22H46O	000661-19-8	91
4			1-Heneicosanol	312	C21H44O	015594-90-8	91
5			1-Tetracosene	336	C24H48	010192-32-2	90



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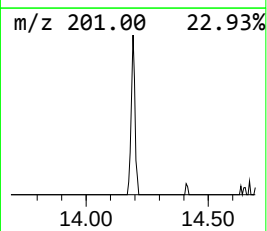
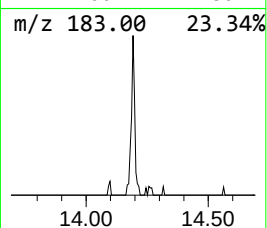
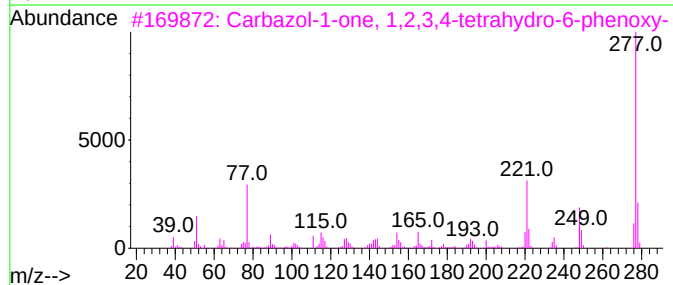
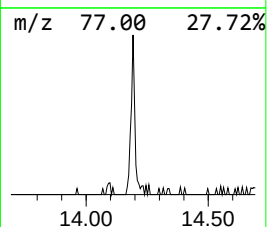
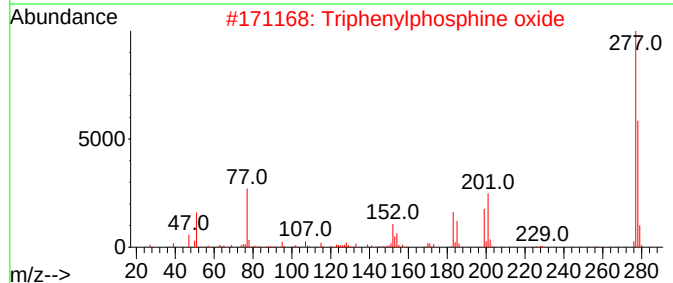
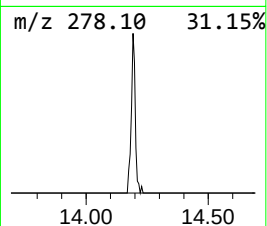
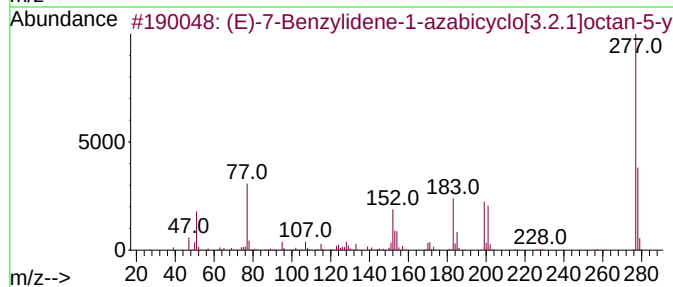
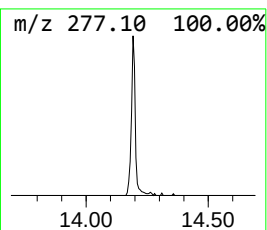
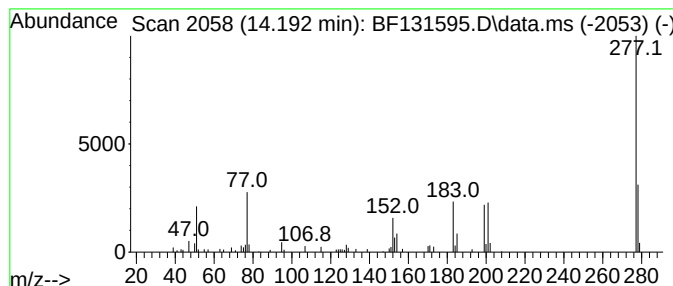
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 5 (E)-7-Benzylidene-1-azabicy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.192	3.17 ng	56809	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	87		
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	80		
3	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	37		
4	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	35		
5	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	27		



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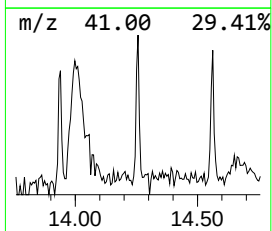
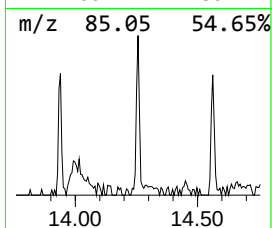
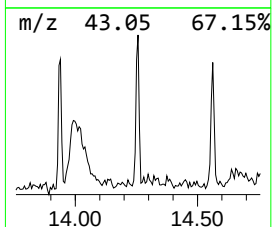
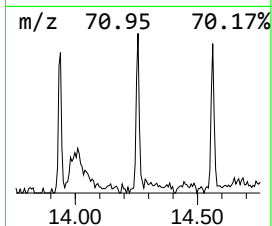
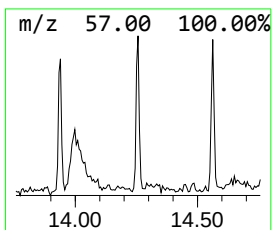
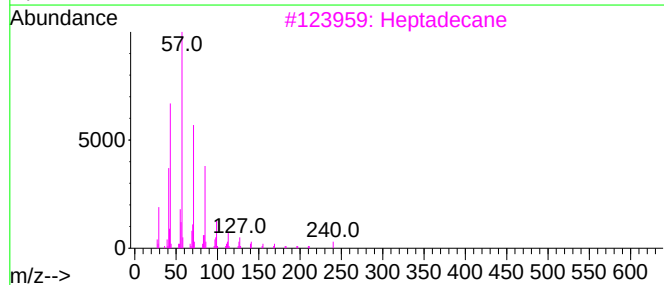
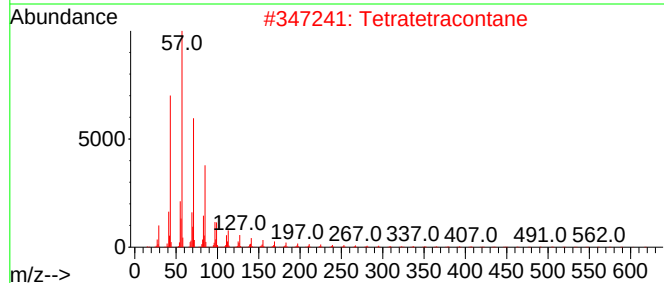
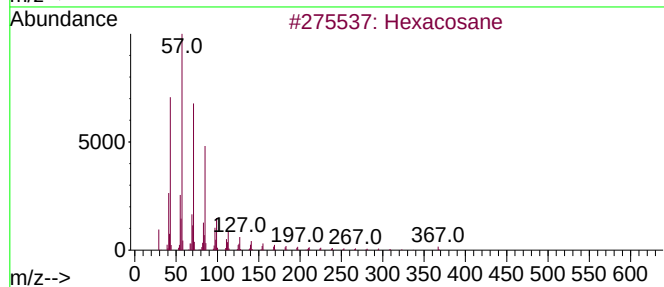
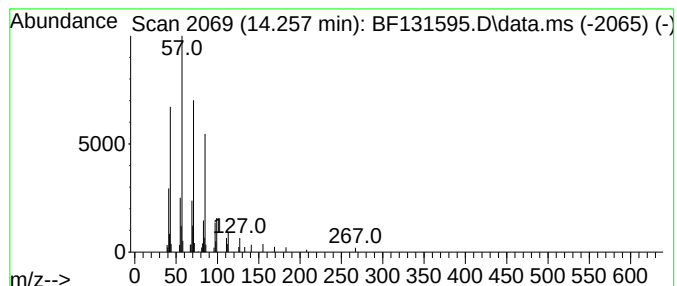
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.257	2.26 ng	40536	Chrysene-d12	14.098

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	91
2		Tetratetracontane	619	C44H90	007098-22-8	91
3		Heptadecane	240	C17H36	000629-78-7	90
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131595.D
Acq On : 12 Dec 2022 16:31
Operator : CG\JU
Sample : N5964-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-518-COMP-01

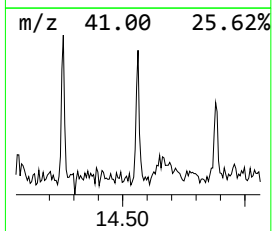
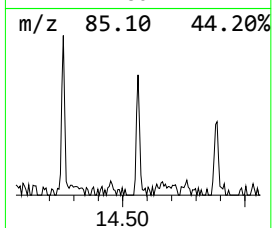
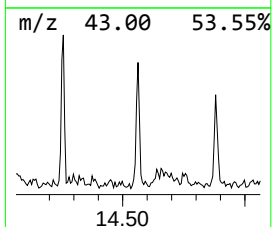
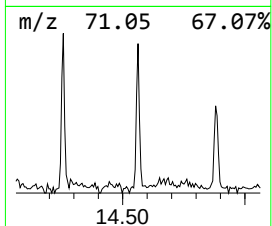
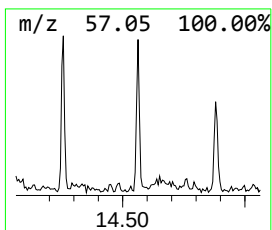
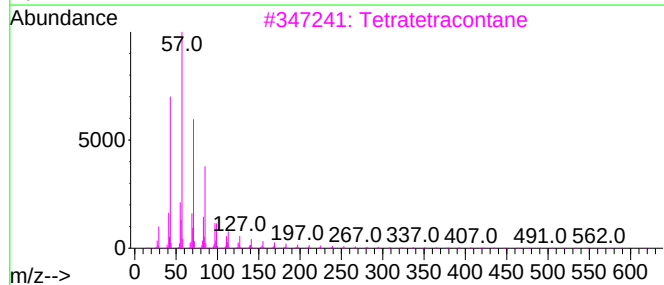
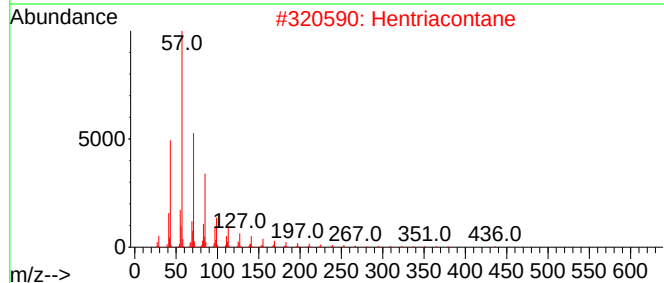
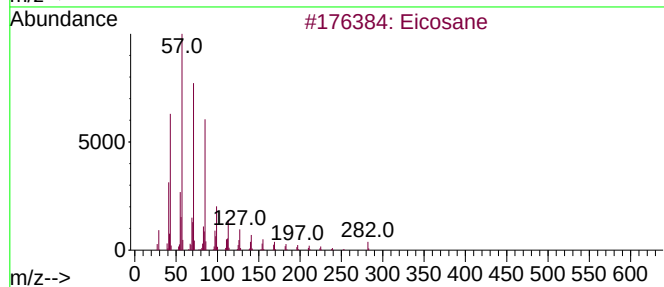
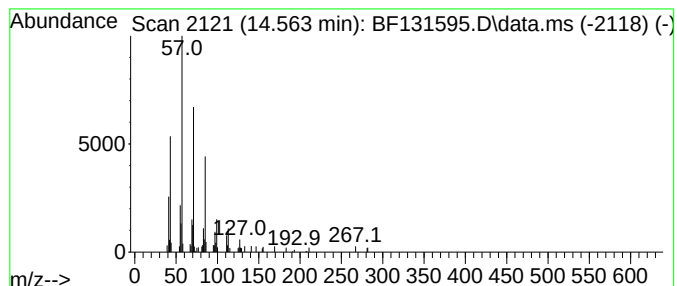
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.563	2.02 ng	36144	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	95
2			Hentriacontane	437	C31H64	000630-04-6	91
3			Tetratetracontane	619	C44H90	007098-22-8	91
4			Hexacosane	366	C26H54	000630-01-3	91
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131595.D
Acq On : 12 Dec 2022 16:31
Operator : CG\JU
Sample : N5964-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-518-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.181	30.9	ng	585779	1	6.893	378984	20.0
2-Pentanone, 4-...	5.104	11.8	ng	223429	1	6.893	378984	20.0
Octacosane	13.939	2.1	ng	37820	5	14.098	358748	20.0
Eicosyl methyl ...	13.998	3.6	ng	63914	5	14.098	358748	20.0
(E)-7-Benzylide...	14.192	3.2	ng	56809	5	14.098	358748	20.0
Hexacosane	14.257	2.3	ng	40536	5	14.098	358748	20.0
Eicosane	14.563	2.0	ng	36144	5	14.098	358748	20.0