

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031925\
 Data File : BF141999.D
 Acq On : 19 Mar 2025 11:47
 Operator : RC/JU
 Sample : Q1590-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20071

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: BF141999.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	19	rVB	850532	1377805	38.43%	5.761%
2	5.492	568	578	583	rBV	1883062	2524257	70.42%	10.554%
3	5.822	630	634	652	rVB	140108	201923	5.63%	0.844%
4	6.498	742	749	754	rBV	1826701	2504653	69.87%	10.473%
5	6.704	780	784	789	rVB	129274	164814	4.60%	0.689%
6	6.875	808	813	820	rBV	741594	953682	26.60%	3.988%
7	7.434	900	908	913	rBV	1251308	1832337	51.11%	7.661%
8	7.898	980	987	990	rBV3	76810	144669	4.04%	0.605%
9	8.157	1025	1031	1038	rBV2	941542	1480827	41.31%	6.192%
10	8.663	1113	1117	1120	rBV	117197	169495	4.73%	0.709%
11	8.751	1128	1132	1135	rBV2	212822	293052	8.17%	1.225%
12	9.233	1209	1214	1218	rBV	2715194	3584798	100.00%	14.989%
13	9.316	1224	1228	1232	rBV2	947627	1633522	45.57%	6.830%
14	9.586	1270	1274	1279	rVB	2342252	3098869	86.44%	12.957%
15	9.792	1306	1309	1312	rBV3	1268661	2087701	58.24%	8.729%
16	15.515	2277	2282	2287	rBV	588339	911214	25.42%	3.810%
17	16.580	2458	2463	2470	rBV	86051	186729	5.21%	0.781%
18	17.833	2669	2676	2686	rVB	231343	621859	17.35%	2.600%
19	17.998	2699	2704	2714	rVB3	55492	144269	4.02%	0.603%

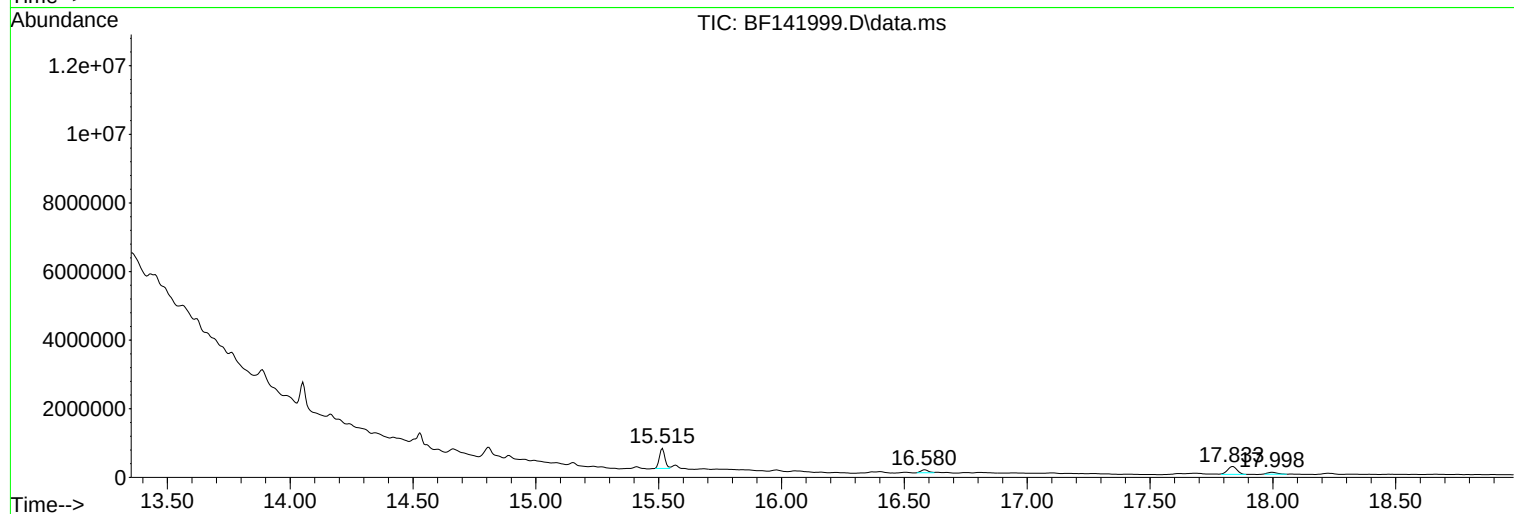
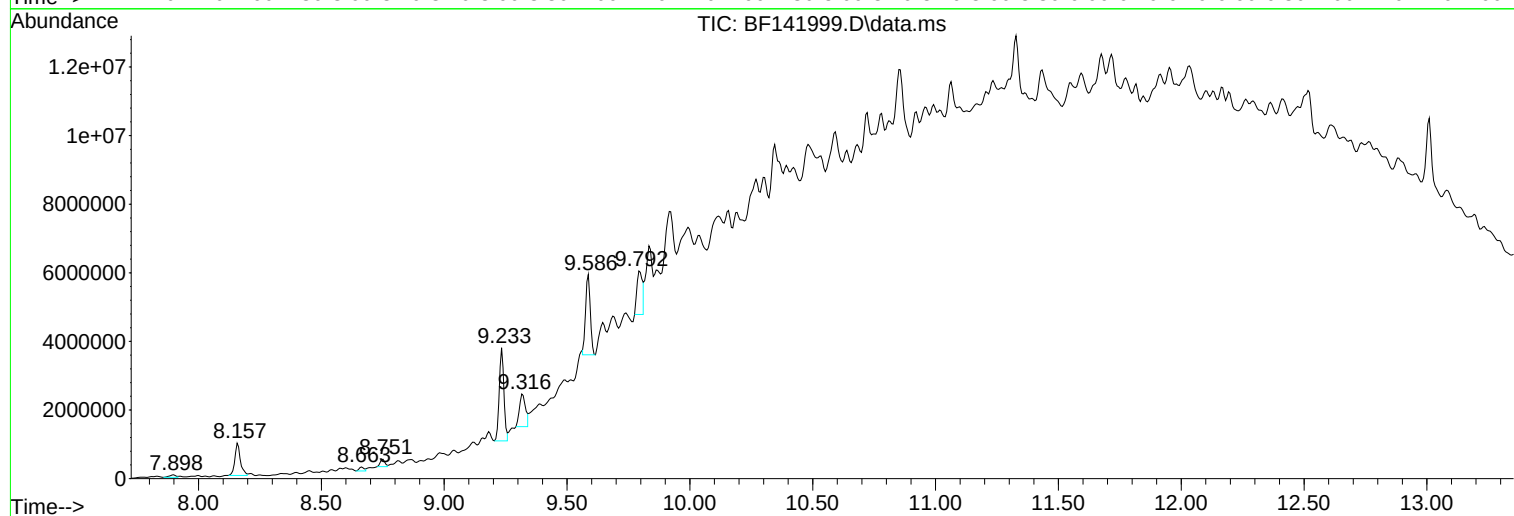
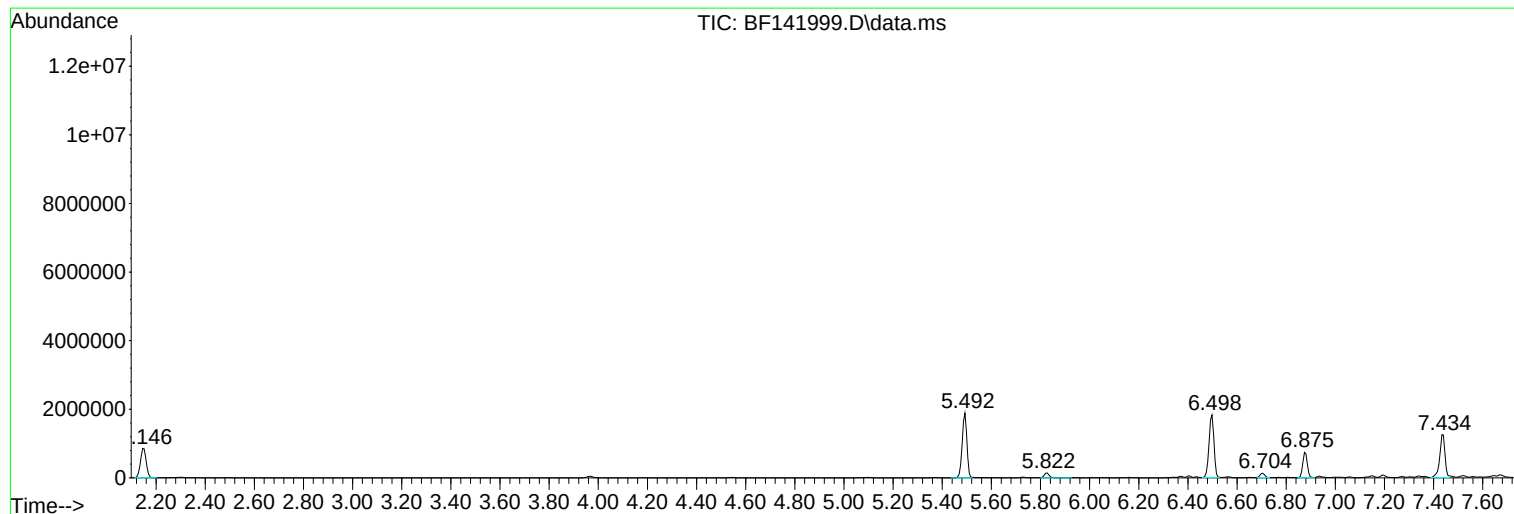
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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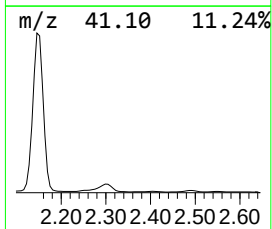
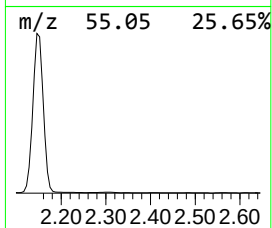
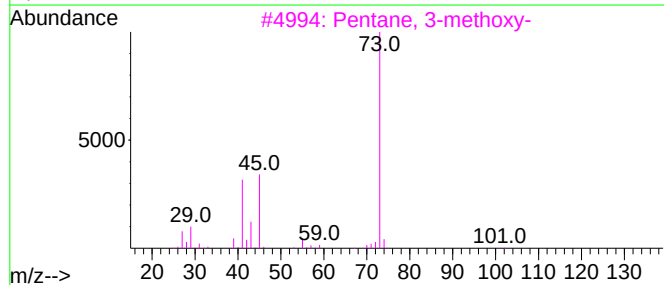
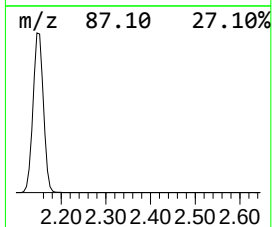
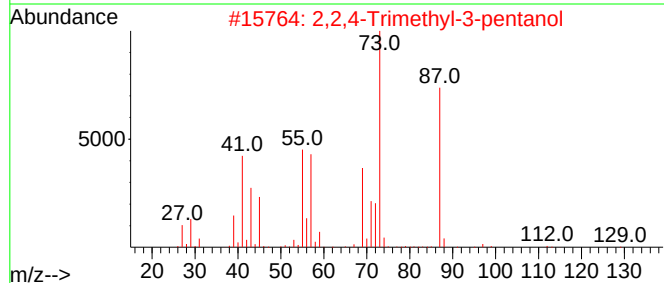
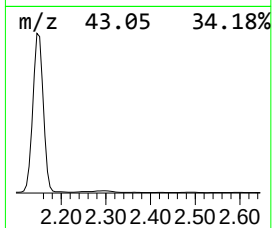
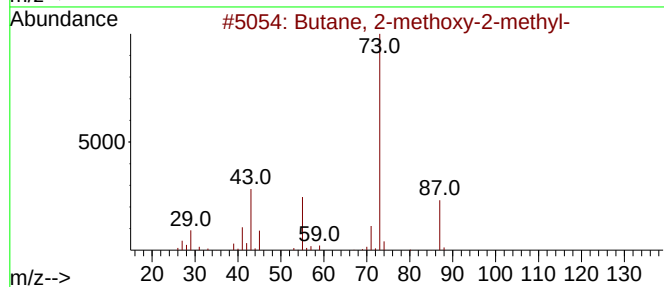
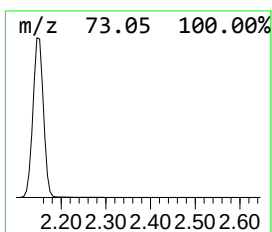
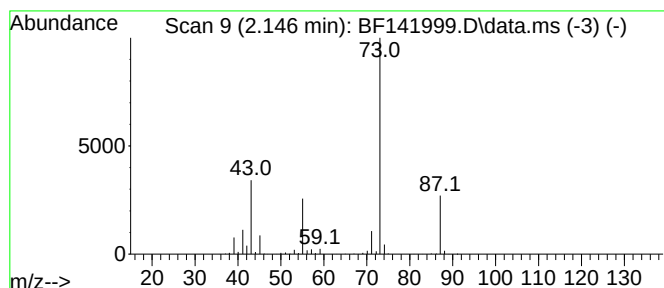
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	28.89 ng	1377810	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			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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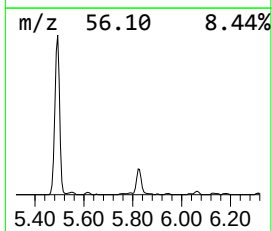
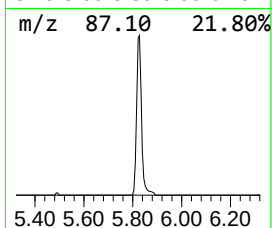
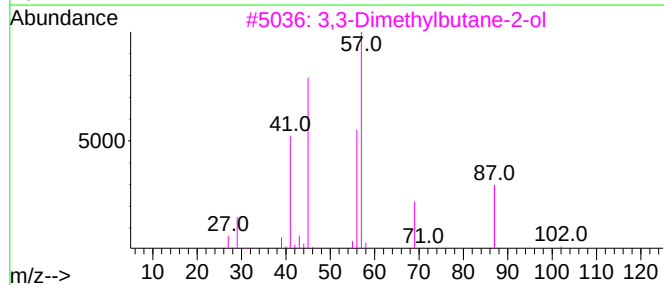
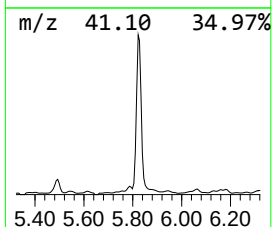
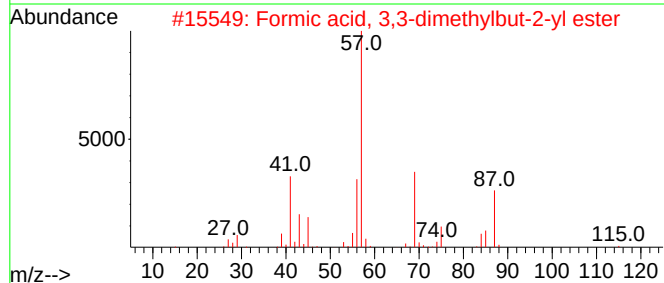
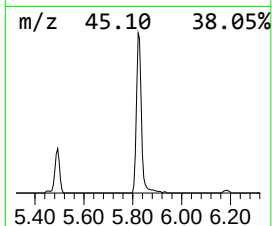
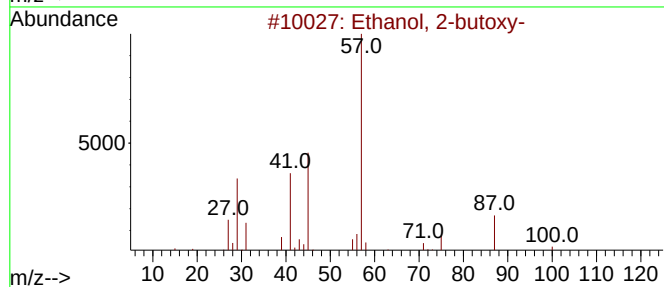
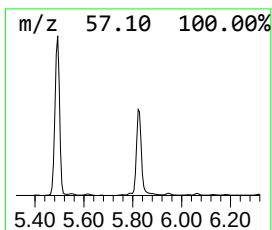
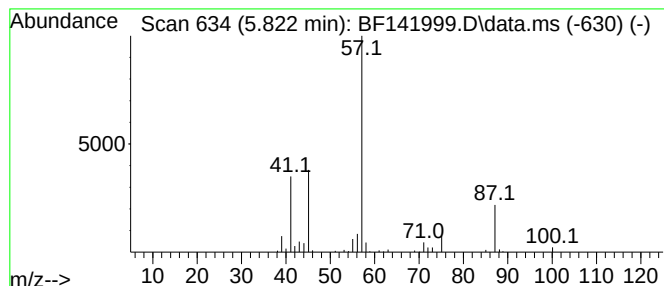
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-butoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.822	4.23 ng	201923	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
2			Formic acid, 3,3-dimethylbut-2-y...	130	C7H14O2	1000368-20-5	50
3			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	33
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	28
5			n-Butyl ether	130	C8H18O	000142-96-1	17



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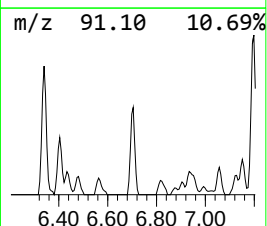
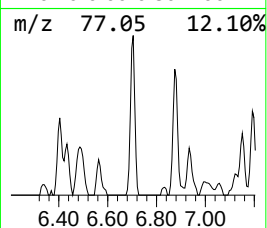
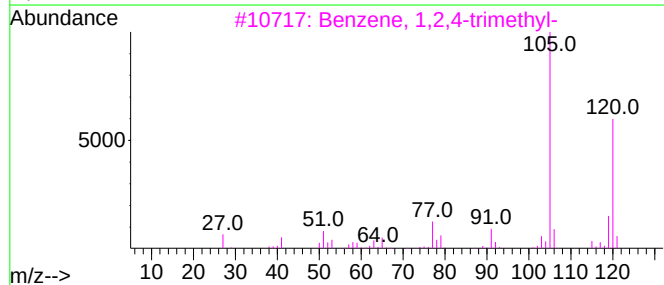
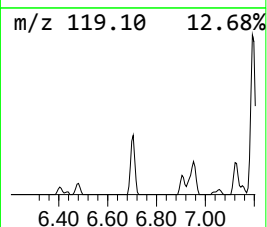
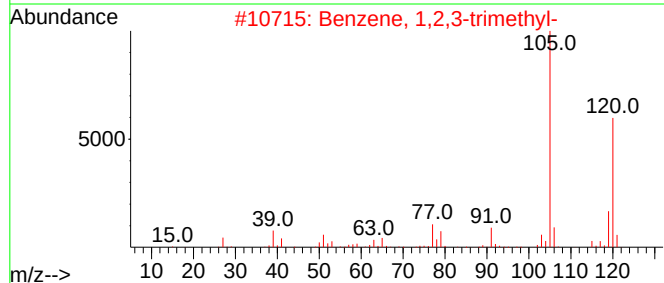
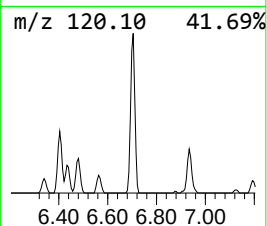
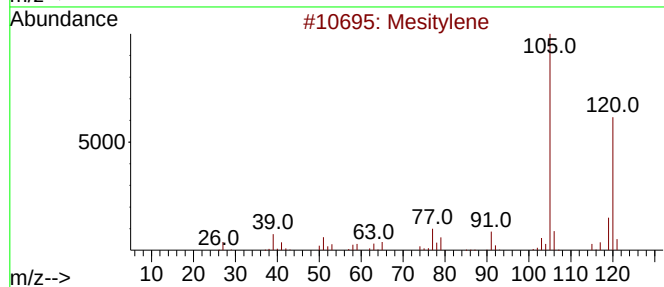
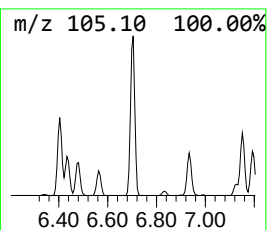
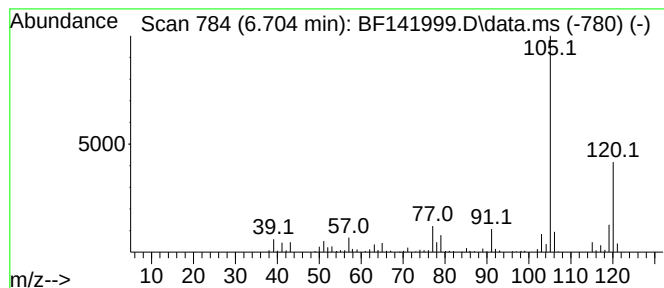
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Mesitylene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.704	3.46 ng	164814	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	97
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90



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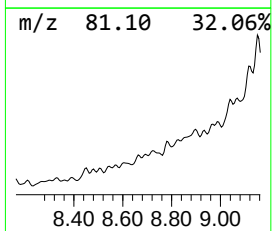
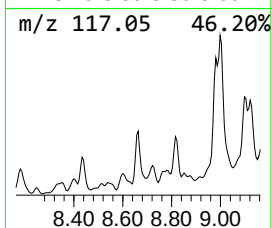
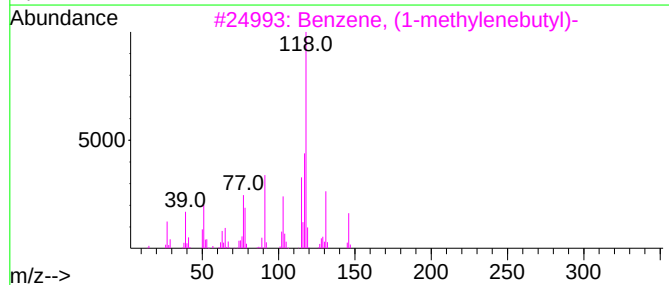
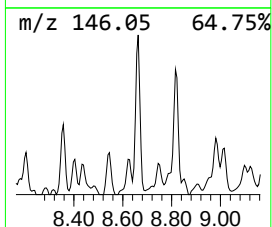
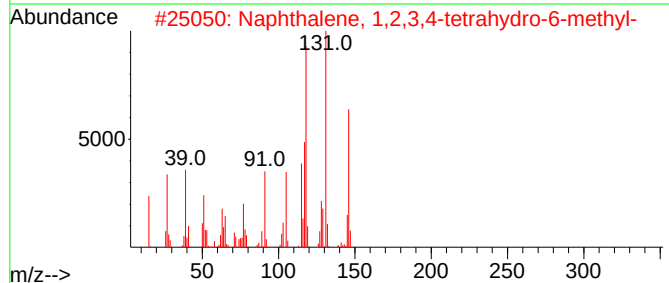
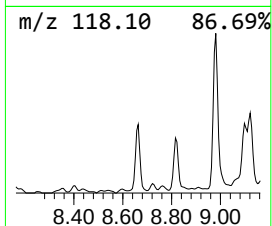
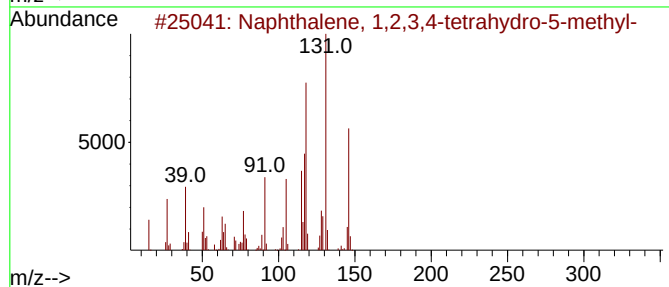
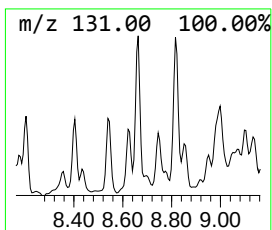
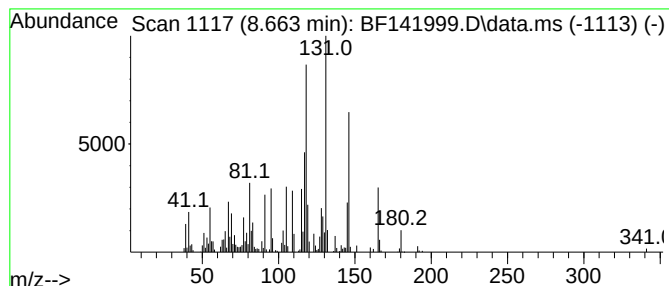
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Naphthalene, 1,2,3,4-tetra... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.663	2.29 ng	169495	Naphthalene-d8	8.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	89
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	86
3			Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	70
4			1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	58
5			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	41



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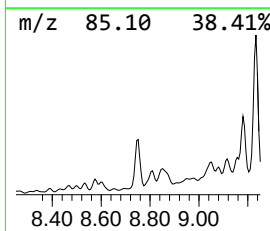
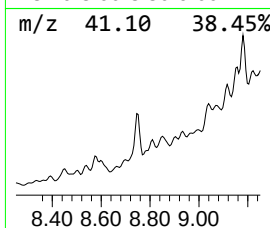
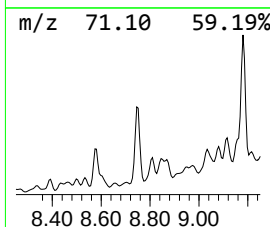
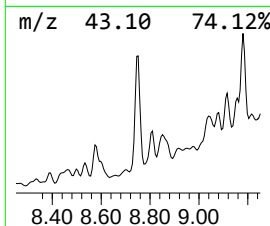
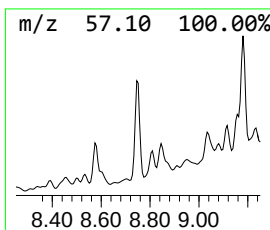
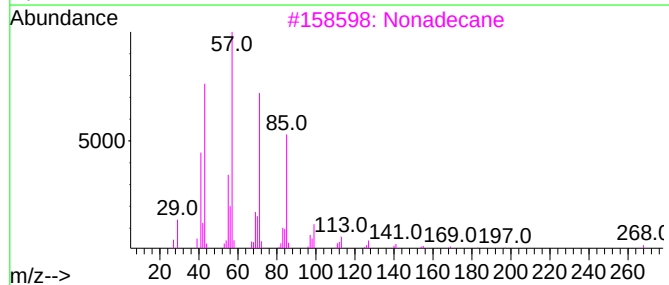
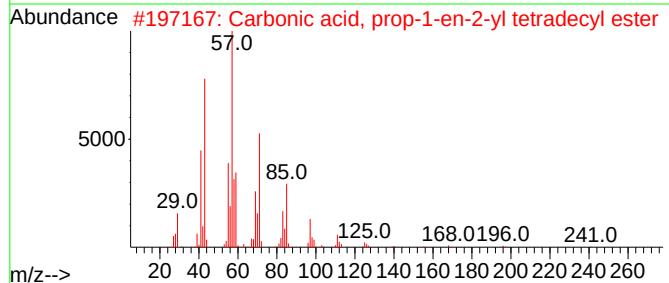
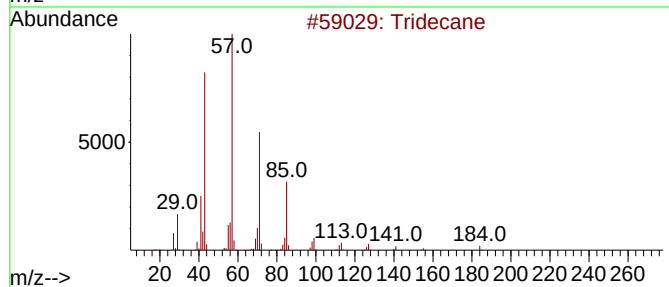
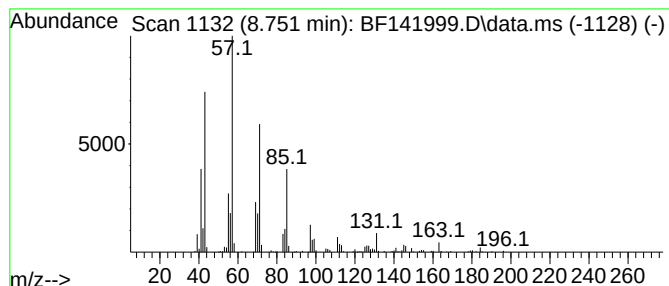
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Tridecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.751	3.96 ng	293052	Naphthalene-d8	8.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	87
2			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	83
3			Nonadecane	268	C19H40	000629-92-5	72
4			Dodecane	170	C12H26	000112-40-3	72
5			Nonane	128	C9H20	000111-84-2	60



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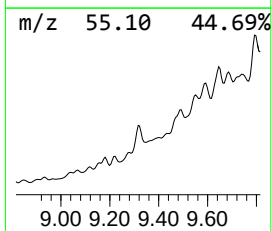
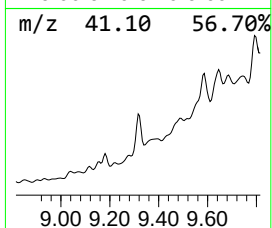
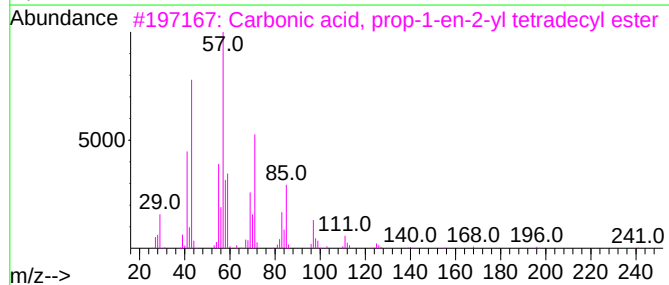
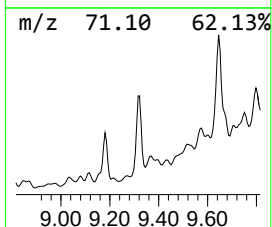
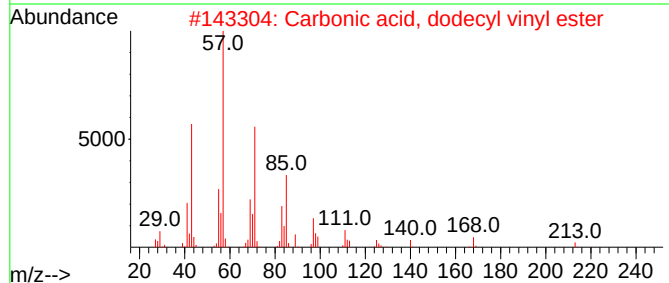
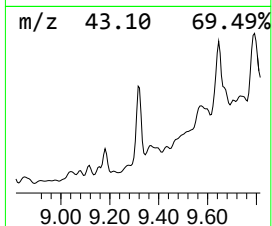
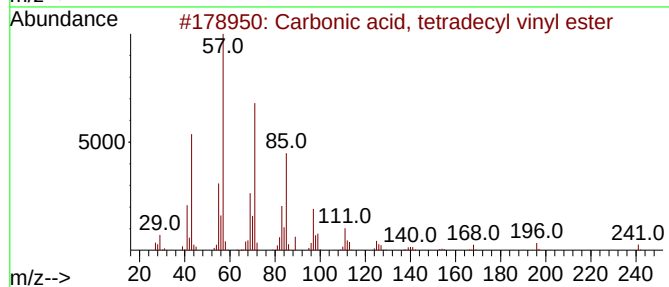
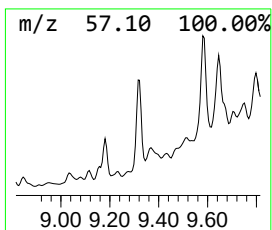
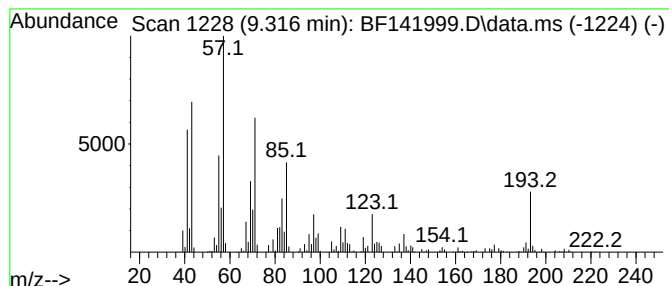
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Carbonic acid, tetradecyl v... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.316	15.65 ng	1633520	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	76
2			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	68
3			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	64
4			Tetradecane	198	C14H30	000629-59-4	64
5			Carbonic acid, tridecyl vinyl ester	270	C16H30O3	1000382-54-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031925\
Data File : BF141999.D
Acq On : 19 Mar 2025 11:47
Operator : RC/JU
Sample : Q1590-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

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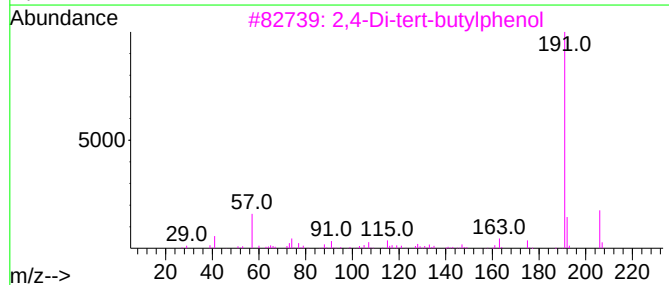
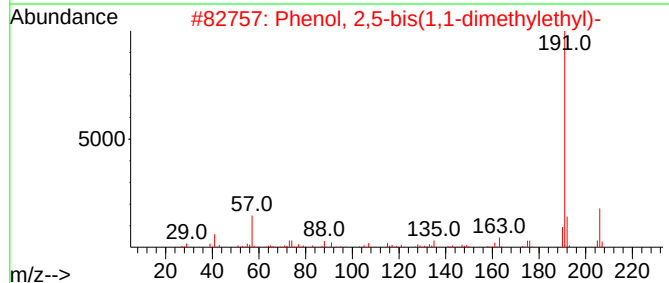
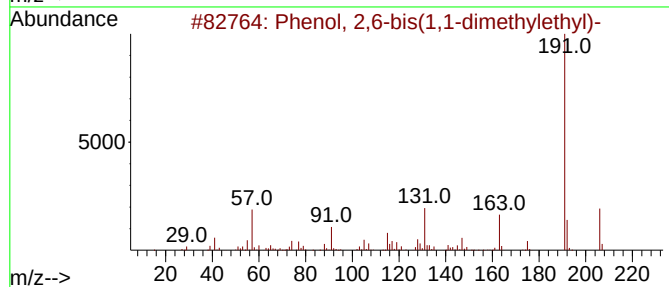
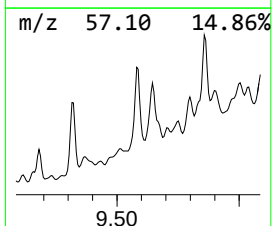
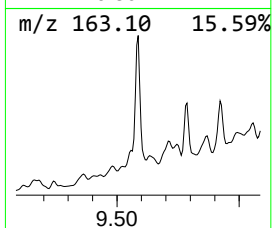
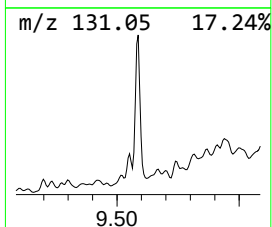
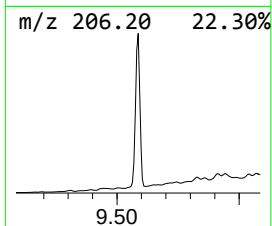
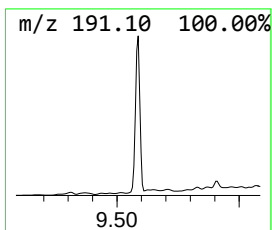
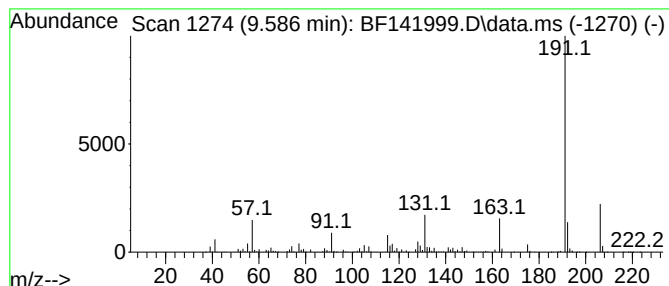
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.586	29.69 ng	3098870	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	94
2			Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	83
3			2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	81
4			3-(4-(tert-Butyl)phenyl)-2-methy...	206	C14H22O	056107-04-1	81
5			Ethyl 4-t-butylbenzoate	206	C13H18O2	005406-57-5	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031925\
Data File : BF141999.D
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Sample : Q1590-02
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Instrument :
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ClientSampleId :
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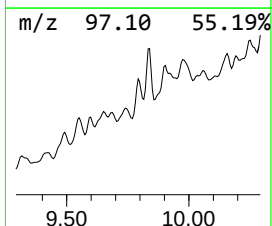
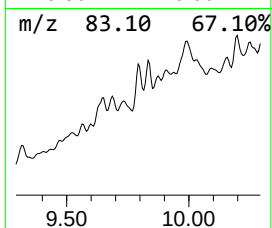
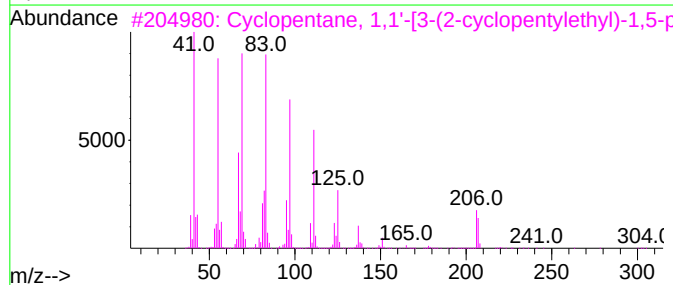
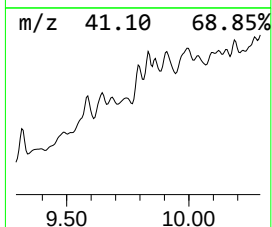
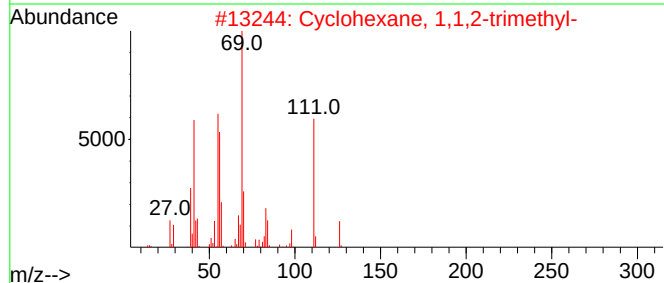
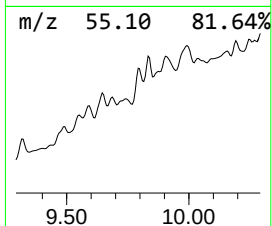
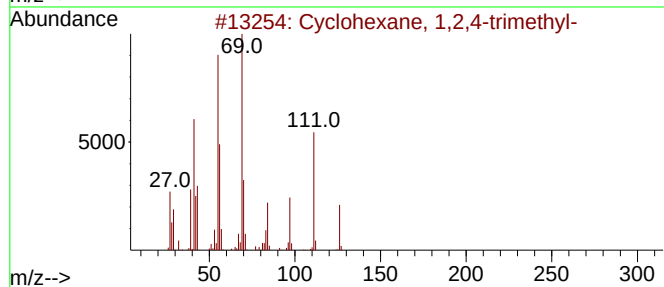
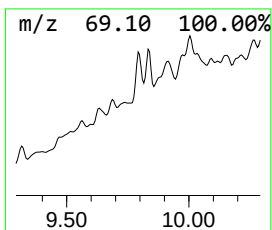
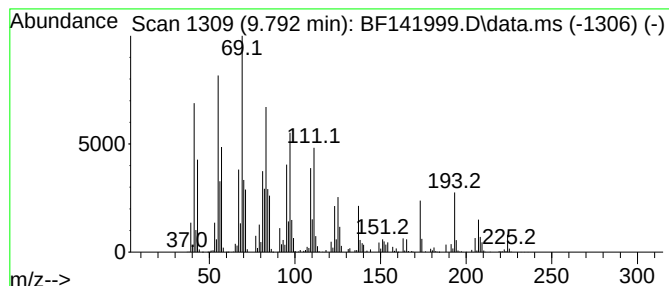
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown9.792 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.792	20.00 ng	2087700	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	38
2			Cyclohexane, 1,1,2-trimethyl-	126	C9H18	007094-26-0	30
3			Cyclopentane, 1,1'-[3-(2-cyclope...	304	C22H40	055255-85-1	30
4			7-Hexadecene, (Z)-	224	C16H32	035507-09-6	30
5			3-Hexadecene, (Z)-	224	C16H32	034303-81-6	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031925\
Data File : BF141999.D
Acq On : 19 Mar 2025 11:47
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Sample : Q1590-02
Misc :
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ClientSampleId :
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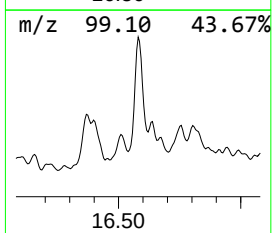
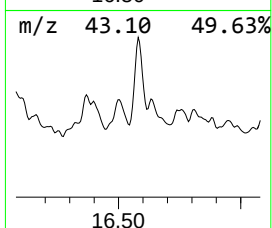
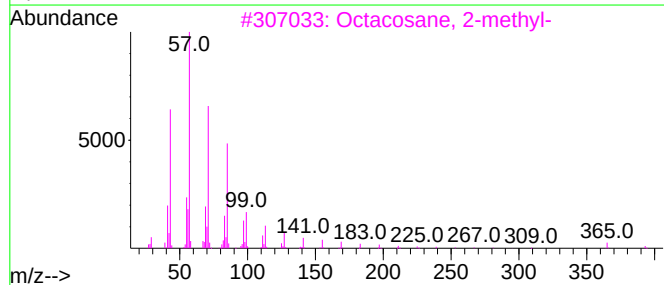
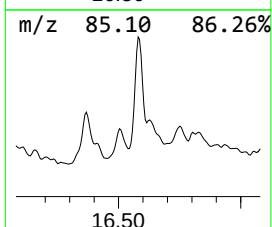
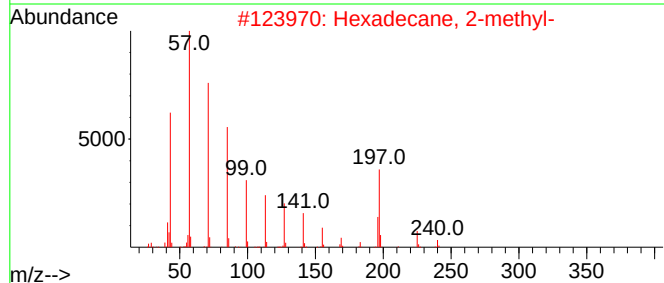
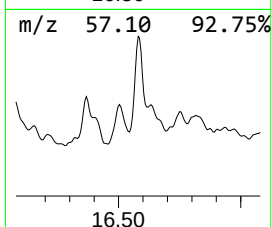
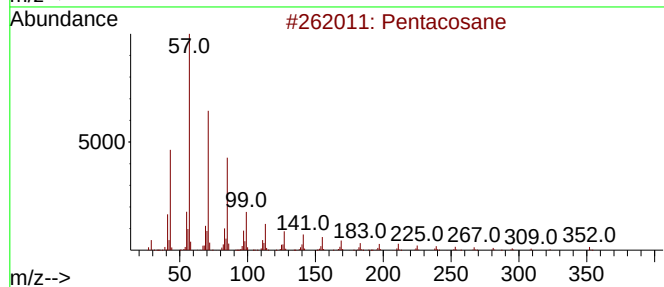
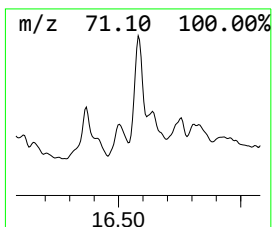
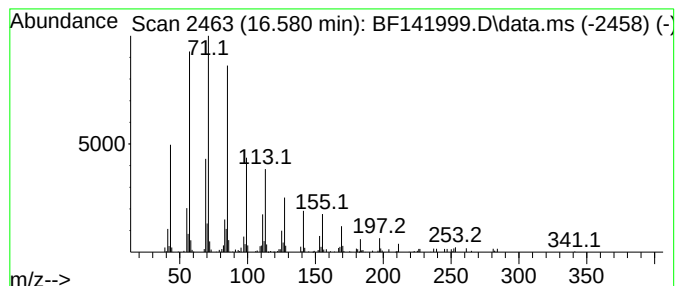
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.580	4.10 ng	186729	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	90
2			Hexadecane, 2-methyl-	240	C17H36	001560-92-5	83
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	78
4			Heptacosane	380	C27H56	000593-49-7	78
5			Octacosane	394	C28H58	000630-02-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031925\
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Acq On : 19 Mar 2025 11:47
Operator : RC/JU
Sample : Q1590-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

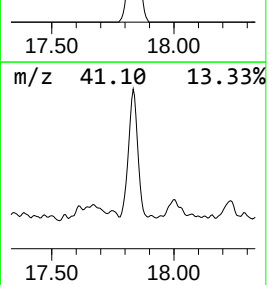
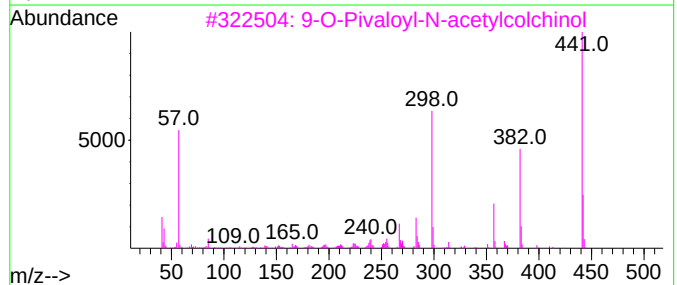
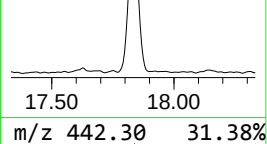
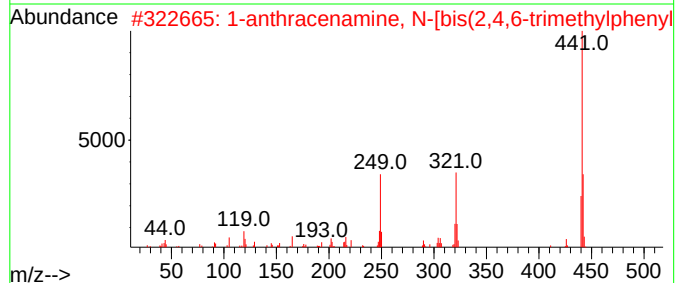
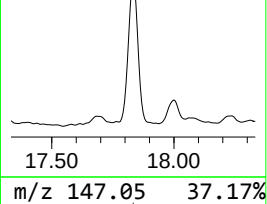
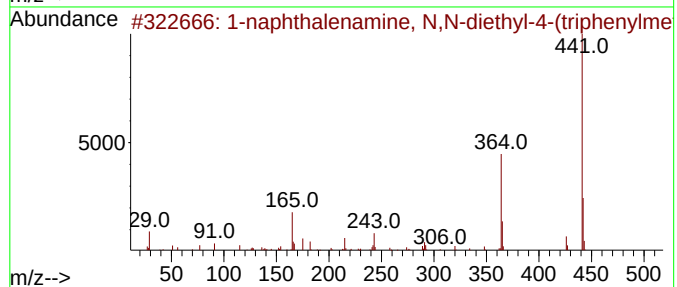
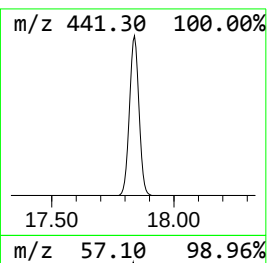
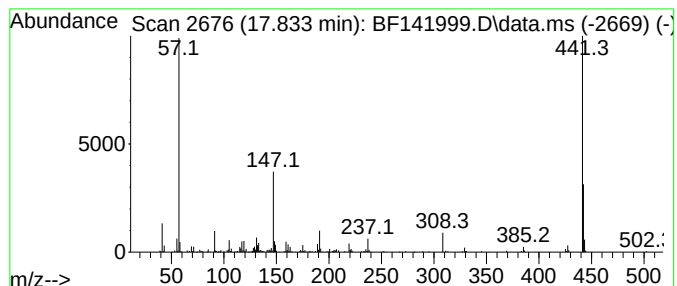
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-naphthalenamine, N,N-diet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.833	13.65 ng	621859	Perylene-d12	15.515		
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-naphthalenamine, N,N-diethyl-4...	441	C33H31N	1000399-30-2	53
2		1-anthracenamine, N-[bis(2,4,6-t...	441	C32H32BN	1000399-30-0	53
3		9-O-Pivaloyl-N-acetylcolchinol	441	C25H31NO6	1000127-10-7	50
4		Silane, diethylheptyloxyoctadecy...	470	C29H62O2Si	1000363-96-0	40
5		Silane, diethyldecyloxypentadecy...	470	C29H62O2Si	1000363-96-6	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031925\
Data File : BF141999.D
Acq On : 19 Mar 2025 11:47
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Sample : Q1590-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

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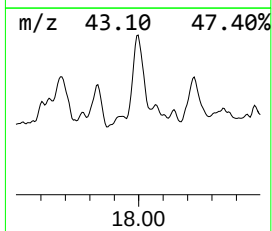
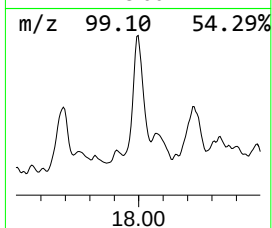
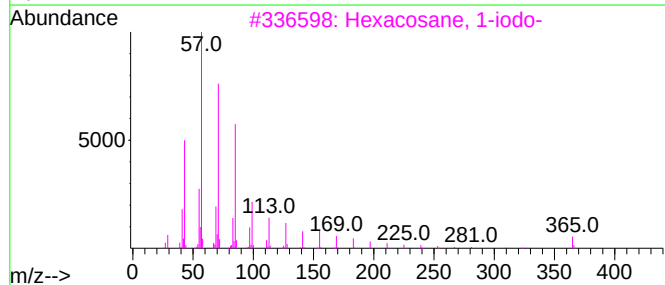
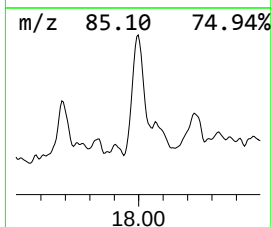
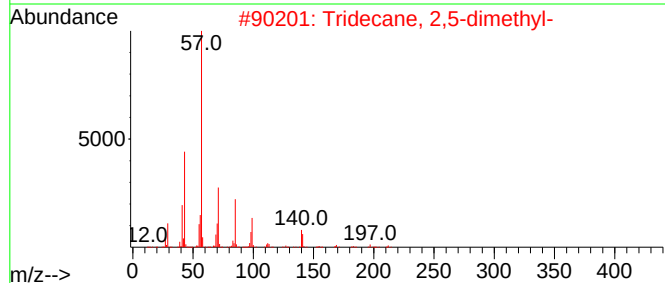
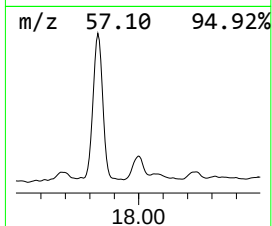
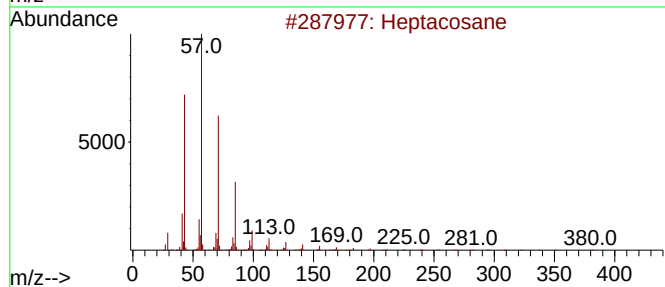
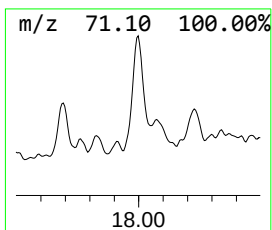
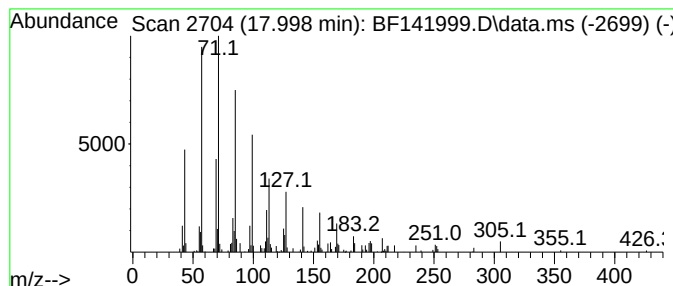
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.997	3.17 ng	144269	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	80
2			Tridecane, 2,5-dimethyl-	212	C15H32	056292-66-1	64
3			Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	58
4			Tridecane, 4,8-dimethyl-	212	C15H32	055030-62-1	58
5			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031925\
Data File : BF141999.D
Acq On : 19 Mar 2025 11:47
Operator : RC/JU
Sample : Q1590-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Ethanol, 2-butoxy-	5.822	4.2	ng	201923	1	6.875	953682	20.0
Mesitylene	6.704	3.5	ng	164814	1	6.875	953682	20.0
Naphthalene, 1,...	8.663	2.3	ng	169495	2	8.157	1480830	20.0
Tridecane	8.751	4.0	ng	293052	2	8.157	1480830	20.0
Carbonic acid, ...	9.316	15.7	ng	1633520	3	9.922	2087700	20.0
Phenol, 2,6-bis...	9.586	29.7	ng	3098870	3	9.922	2087700	20.0
unknown9.792	9.792	20.0	ng	2087700	3	9.922	2087700	20.0
Pentacosane	16.580	4.1	ng	186729	6	15.515	911214	20.0
1-naphthalenami...	17.833	13.7	ng	621859	6	15.515	911214	20.0
Heptacosane	17.997	3.2	ng	144269	6	15.515	911214	20.0