

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072225\
 Data File : BF143202.D
 Acq On : 22 Jul 2025 21:48
 Operator : RC/JU
 Sample : Q2649-13
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-4

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-BF071725.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF143202.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.299	11	18	27	rVB	545471	882524	50.25%	4.865%
2	5.198	502	511	519	rBV	185437	261844	14.91%	1.443%
3	5.598	573	579	585	rBV	1141595	1512829	86.14%	8.339%
4	6.592	742	748	754	rBV	1289827	1756227	100.00%	9.681%
5	6.969	806	812	817	rBV	509596	645953	36.78%	3.561%
6	7.522	898	906	911	rBV	778569	1008058	57.40%	5.557%
7	7.769	944	948	952	rBV	21797	25698	1.46%	0.142%
8	8.245	1024	1029	1038	rBV	633242	798641	45.47%	4.402%
9	8.457	1060	1065	1068	rBV	18453	25814	1.47%	0.142%
10	9.322	1206	1212	1217	rBV	1309667	1646932	93.78%	9.078%
11	9.398	1221	1225	1231	rVB	23954	31592	1.80%	0.174%
12	9.675	1266	1272	1276	rBV2	10478	18636	1.06%	0.103%
13	9.933	1311	1316	1320	rBV	30461	38938	2.22%	0.215%
14	10.004	1323	1328	1333	rVB	581152	718824	40.93%	3.962%
15	10.410	1391	1397	1404	rBV2	90414	165604	9.43%	0.913%
16	10.710	1443	1448	1456	rVV	245738	302006	17.20%	1.665%
17	10.792	1456	1462	1472	rVV	658202	869228	49.49%	4.791%
18	10.904	1477	1481	1489	rBV3	17811	31383	1.79%	0.173%
19	11.022	1497	1501	1506	rVB	31483	38308	2.18%	0.211%
20	11.145	1518	1522	1534	rVV	59286	89995	5.12%	0.496%
21	11.351	1554	1557	1561	rBV2	12015	18475	1.05%	0.102%
22	11.486	1575	1580	1593	rVB	465021	630108	35.88%	3.473%
23	11.586	1593	1597	1603	rBV3	23035	31899	1.82%	0.176%
24	11.780	1626	1630	1634	rBV	18075	29535	1.68%	0.163%
25	11.933	1652	1656	1662	rBV	81882	139166	7.92%	0.767%
26	12.010	1663	1669	1682	rVV2	315870	561682	31.98%	3.096%
27	12.716	1780	1789	1799	rBV3	570496	1513424	86.17%	8.342%
28	12.792	1800	1802	1812	rVB2	99854	159815	9.10%	0.881%
29	13.069	1844	1849	1855	rVB	1208715	1595844	90.87%	8.797%
30	13.610	1938	1941	1944	rBV	34617	40945	2.33%	0.226%
31	13.910	1986	1992	1997	rBV2	198860	413110	23.52%	2.277%
32	13.963	1998	2001	2012	rVB3	144620	257095	14.64%	1.417%
33	14.127	2024	2029	2036	rVB	538726	705974	40.20%	3.892%
34	14.992	2172	2176	2184	rVB	484400	664671	37.85%	3.664%
35	15.639	2281	2286	2294	rBV	318083	510438	29.06%	2.814%

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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

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

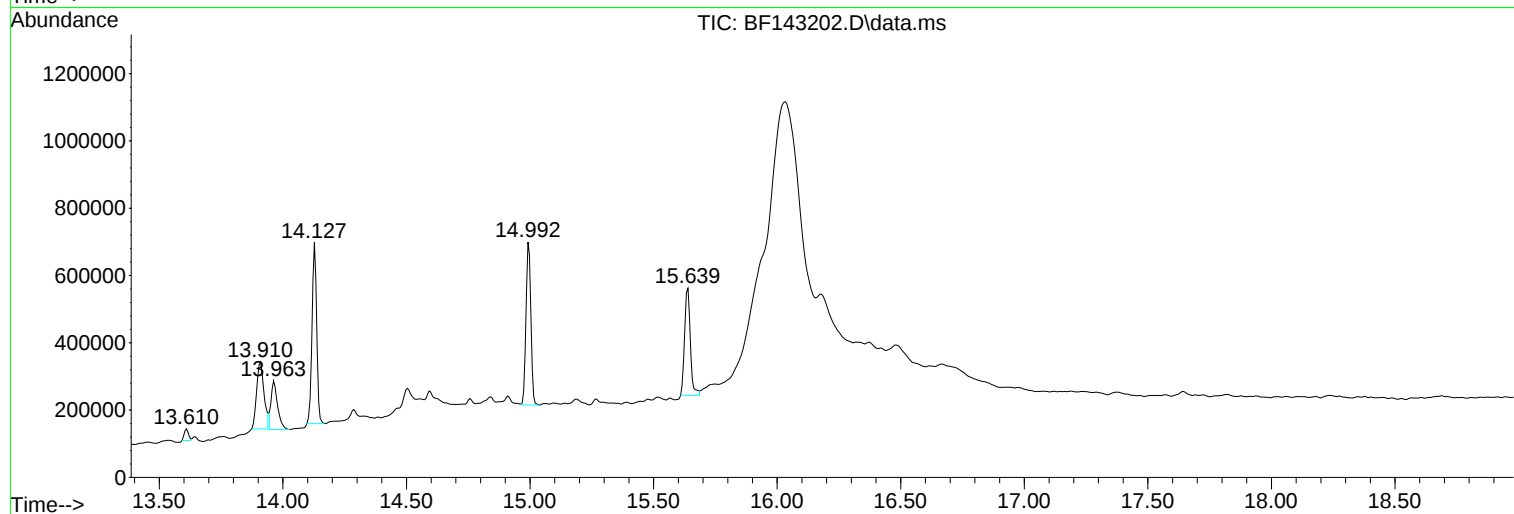
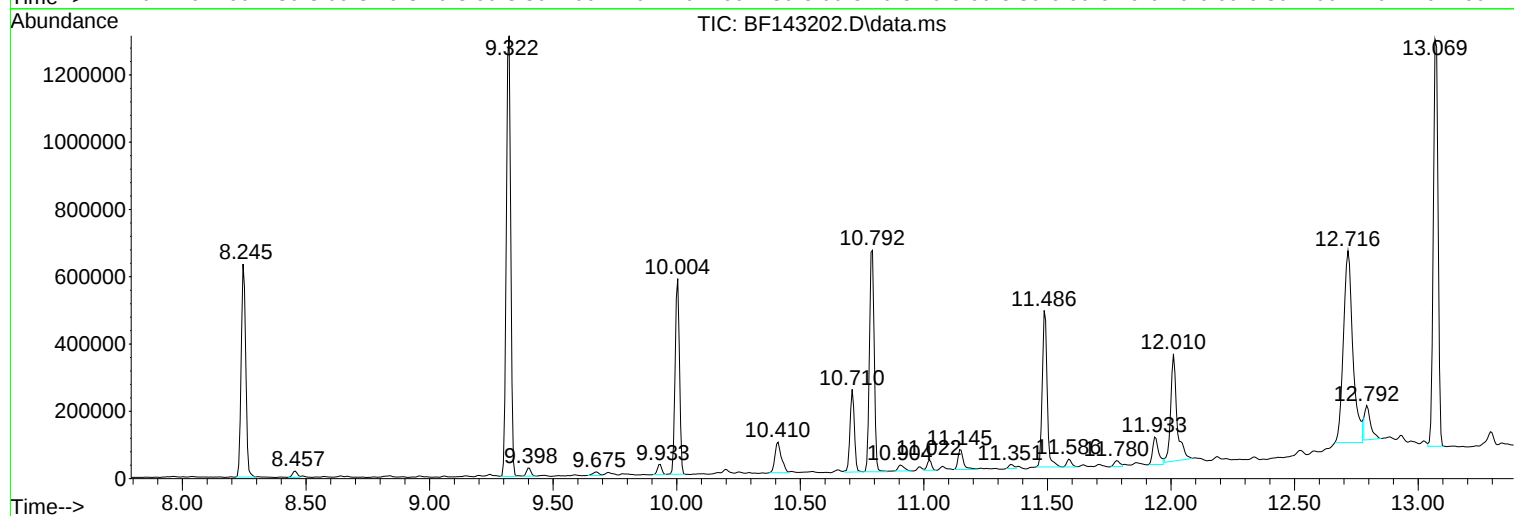
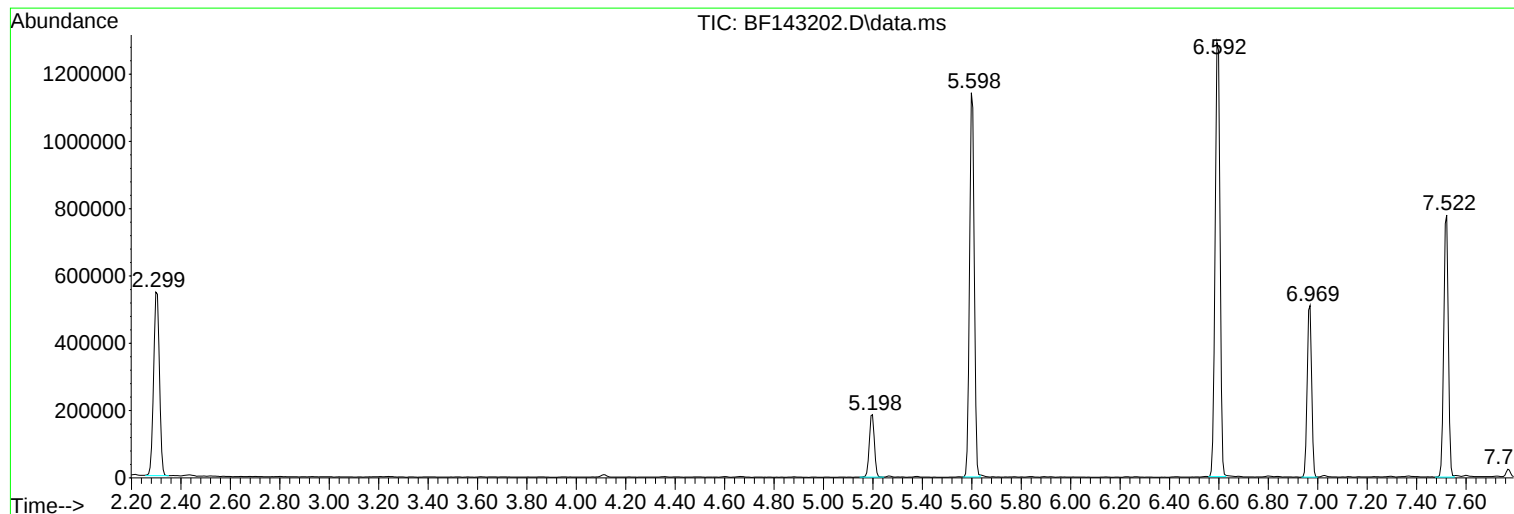
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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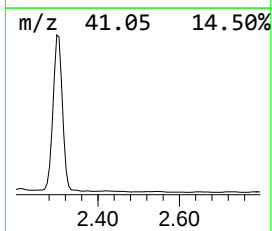
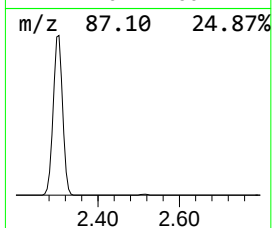
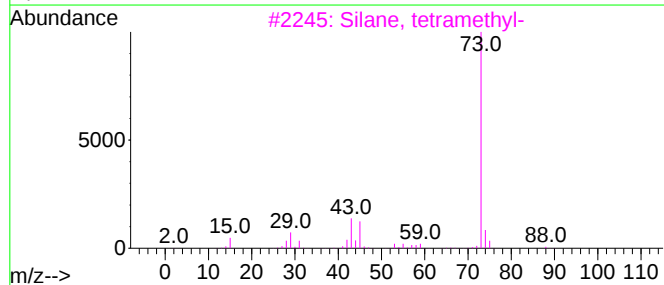
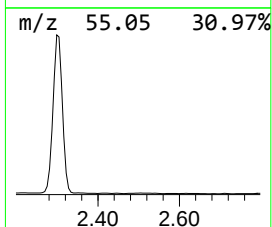
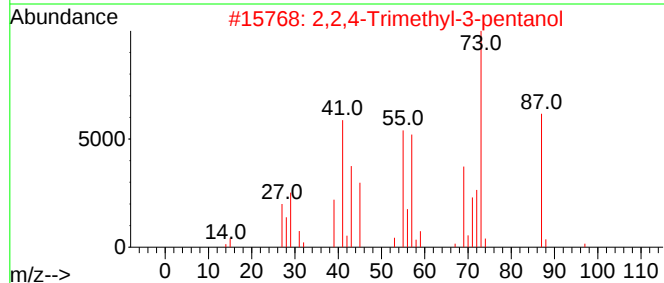
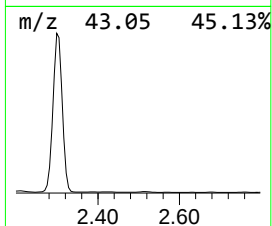
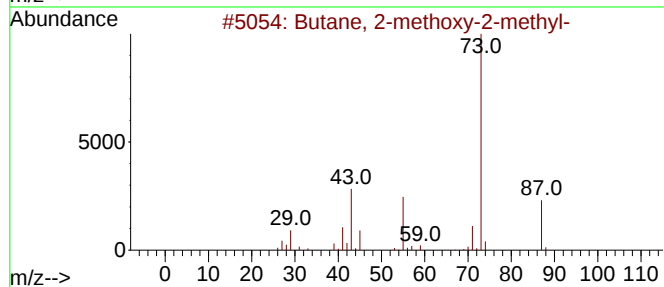
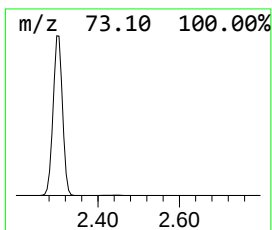
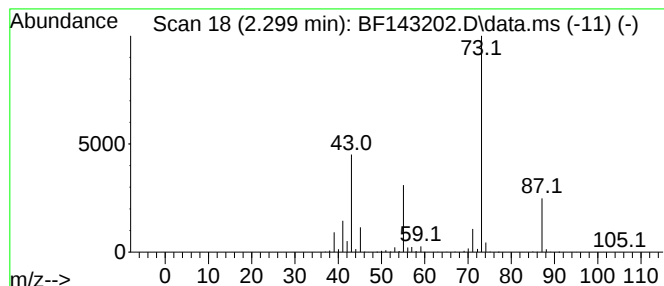
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.299	27.32 ng	882524	1,4-Dichlorobenzene-d4	6.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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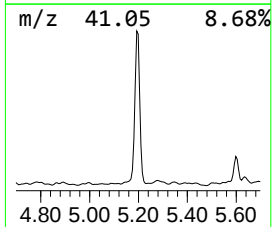
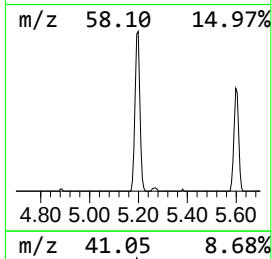
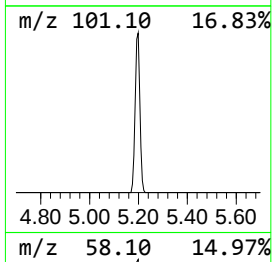
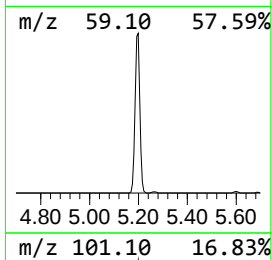
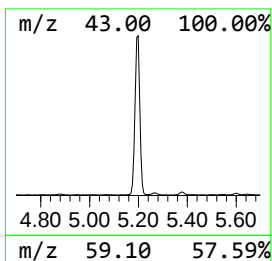
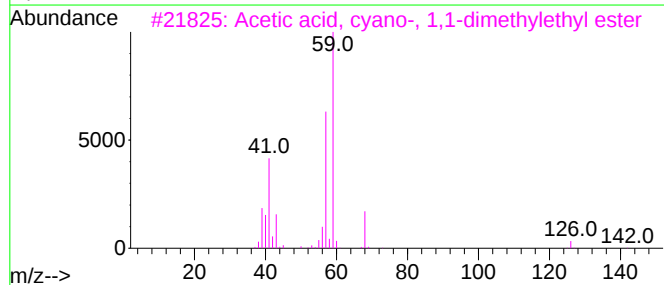
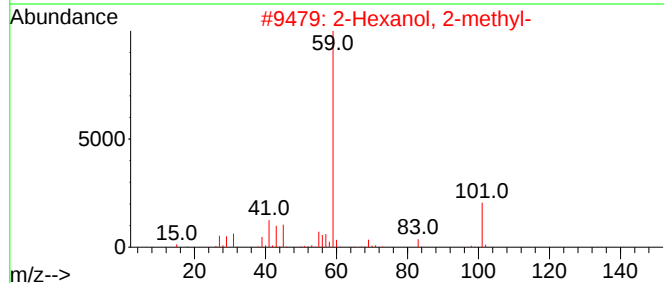
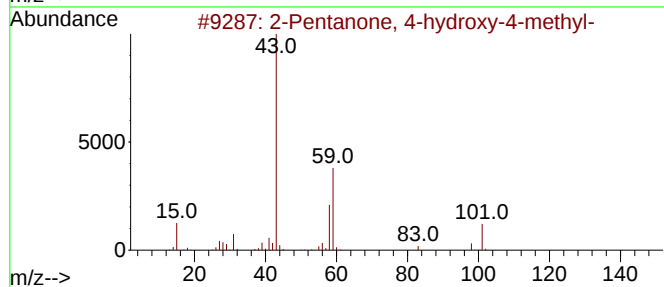
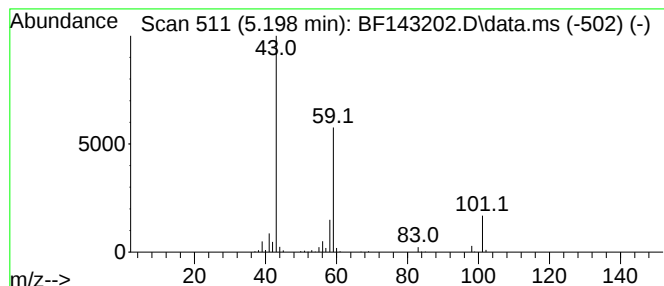
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.198	8.11 ng	261844	1,4-Dichlorobenzene-d4	6.969

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10



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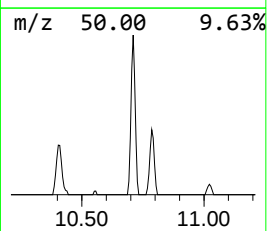
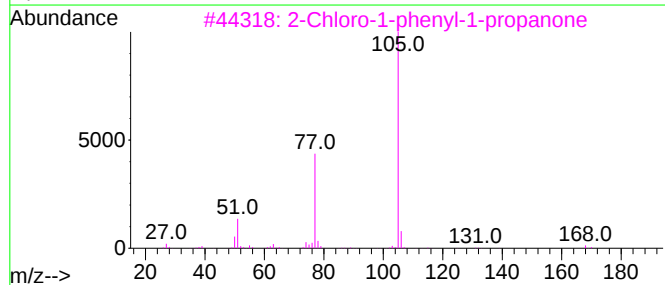
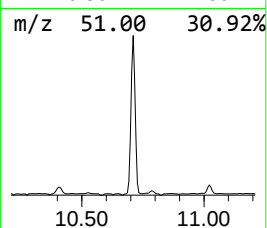
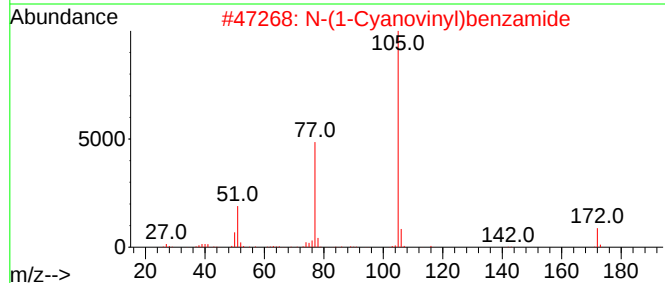
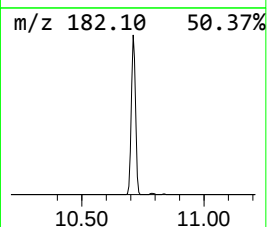
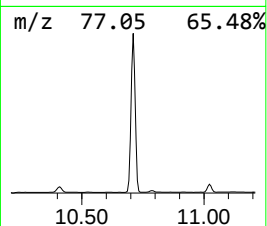
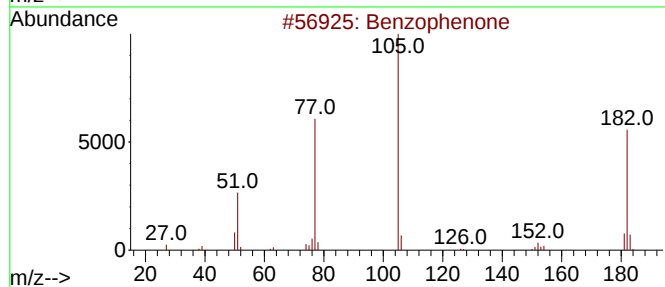
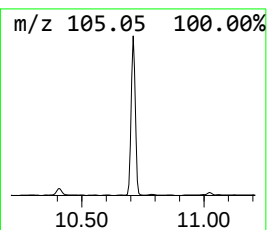
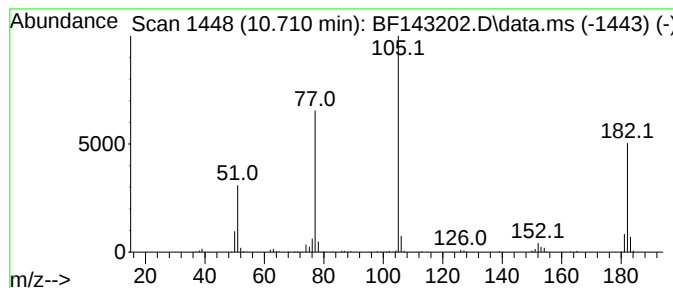
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.710	8.40 ng	302006	Acenaphthene-d10	10.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	50
3			2-Chloro-1-phenyl-1-propanone	168	C9H9ClO	006084-17-9	50
4			2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	50
5			1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	50



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Misc :
ALS Vial : 15 Sample Multiplier: 1

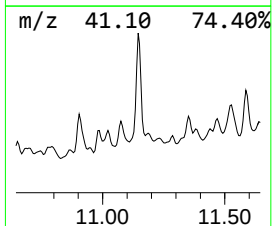
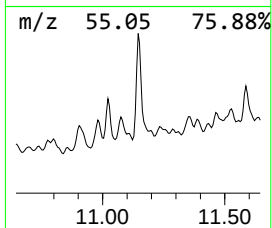
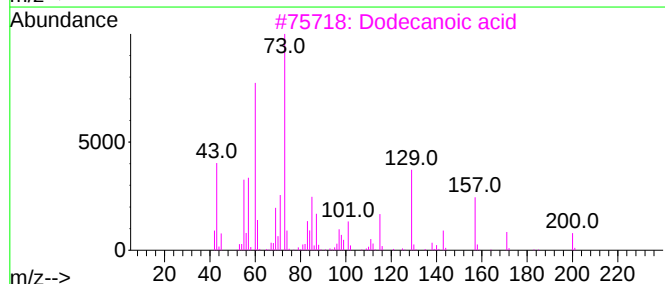
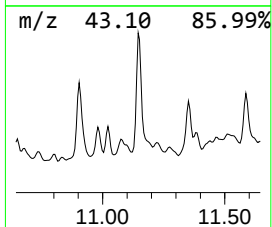
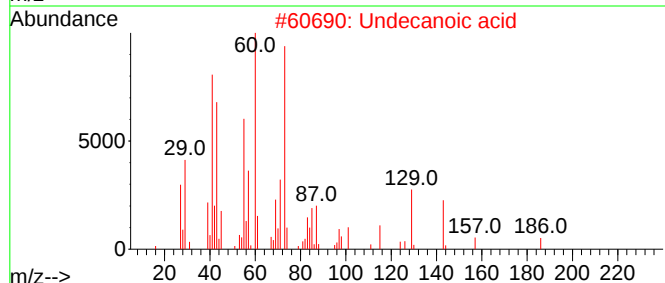
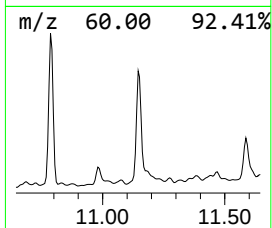
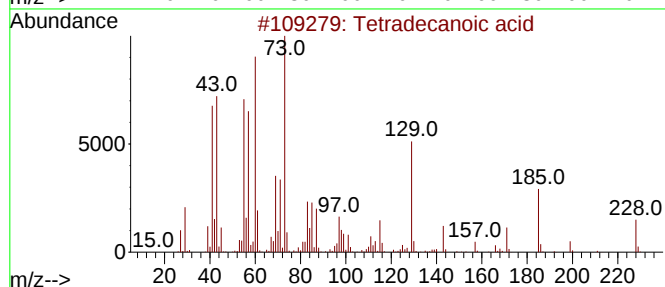
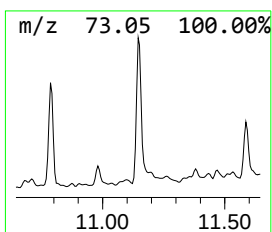
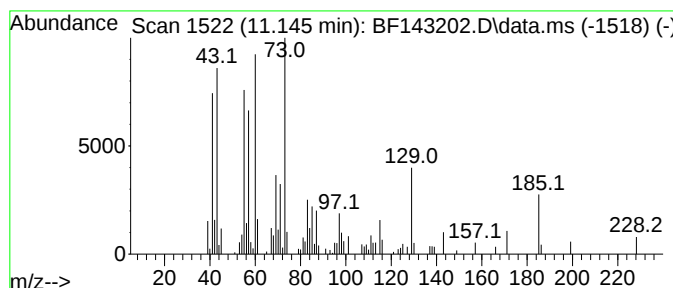
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Peak Number 4 Tetradecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.145	2.86 ng	89995	Phenanthrene-d10		11.486	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Tetradecanoic acid		228	C14H28O2	000544-63-8	95
2	Undecanoic acid		186	C11H22O2	000112-37-8	86
3	Dodecanoic acid		200	C12H24O2	000143-07-7	59
4	n-Decanoic acid		172	C10H20O2	000334-48-5	58
5	Tridecanoic acid		214	C13H26O2	000638-53-9	53



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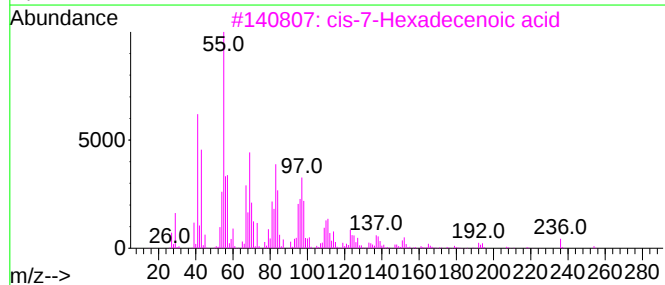
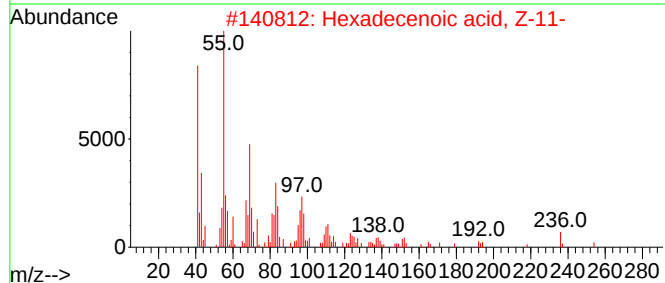
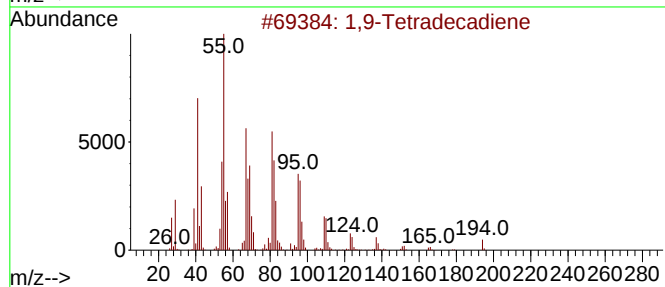
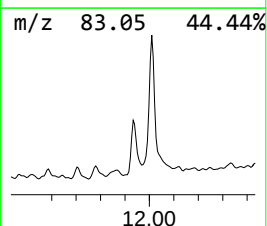
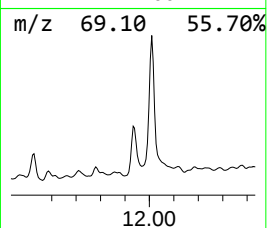
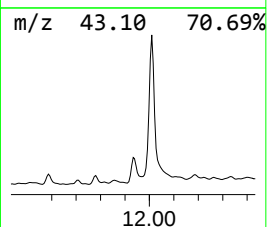
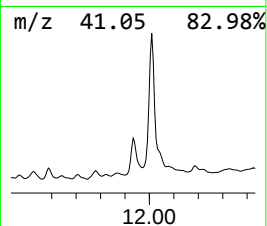
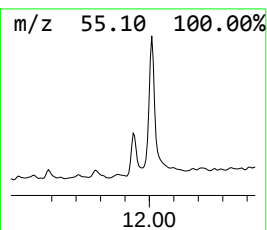
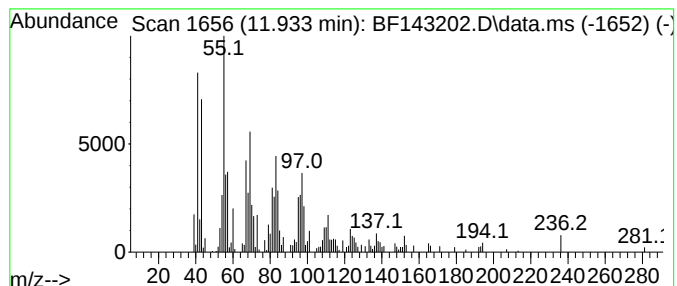
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1,9-Tetradecadiene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	4.42 ng	139166	Phenanthrene-d10	11.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,9-Tetradecadiene	194	C14H26	112929-06-3	83
2			Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	83
3			cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	74
4			(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	68
5			Palmitoleic acid	254	C16H30O2	000373-49-9	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072225\
Data File : BF143202.D
Acq On : 22 Jul 2025 21:48
Operator : RC/JU
Sample : Q2649-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-4

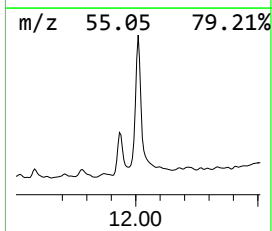
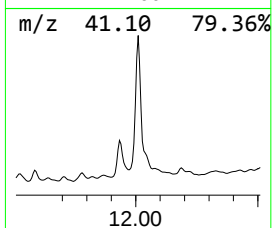
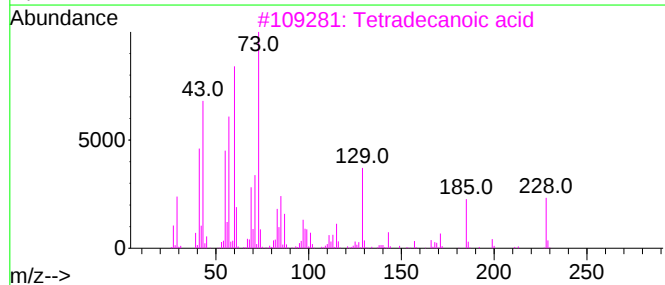
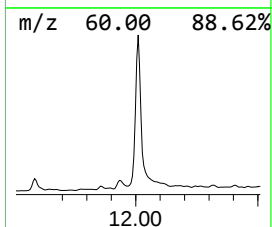
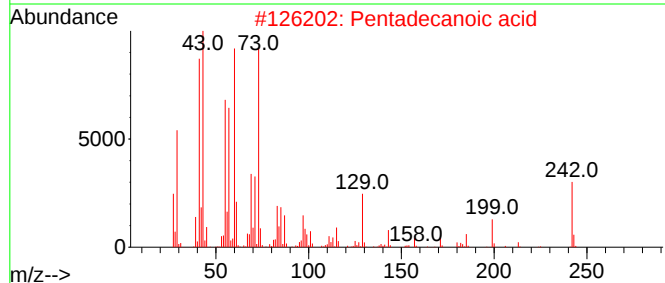
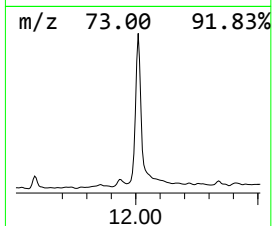
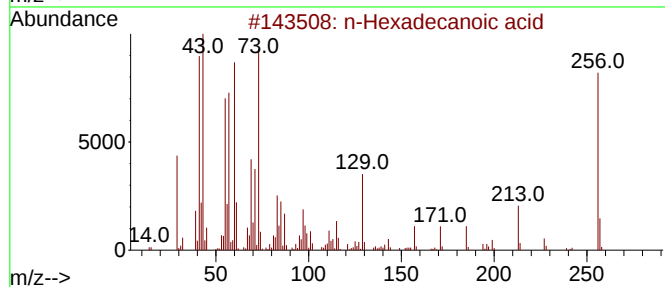
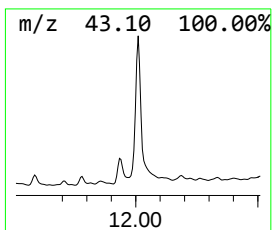
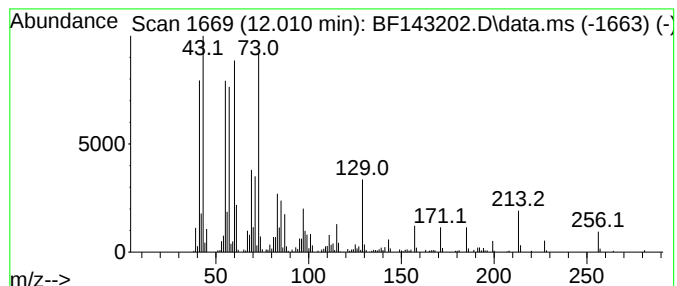
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	17.83 ng	561682	Phenanthrene-d10	11.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072225\
Data File : BF143202.D
Acq On : 22 Jul 2025 21:48
Operator : RC/JU
Sample : Q2649-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

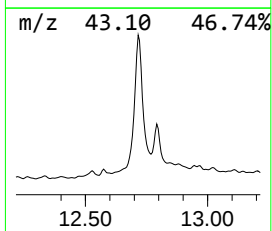
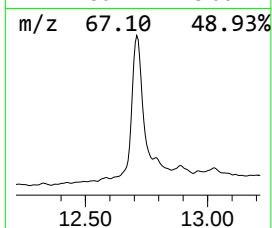
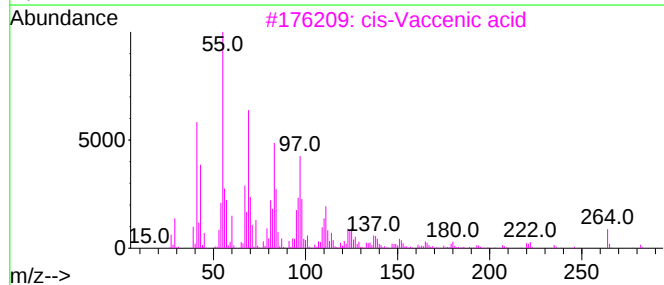
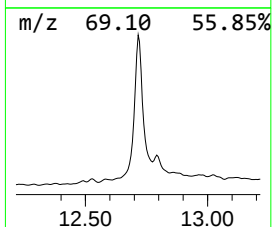
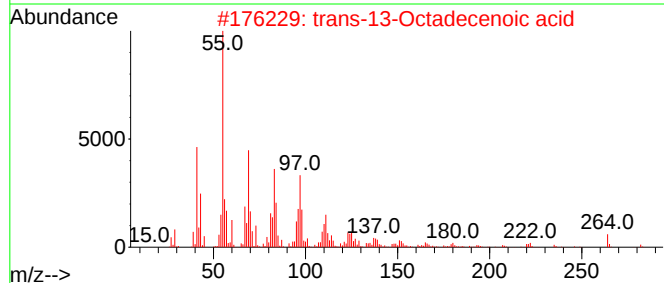
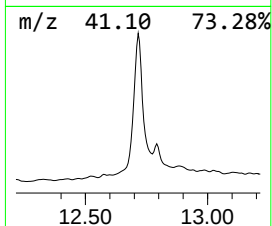
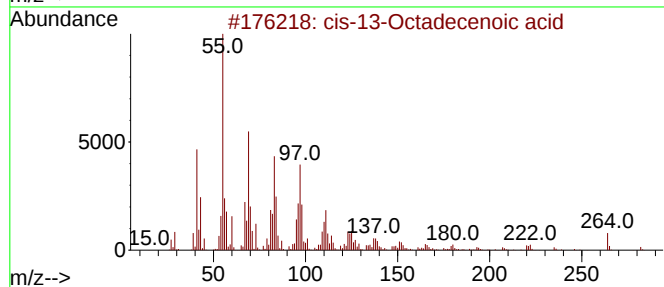
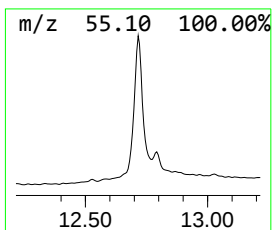
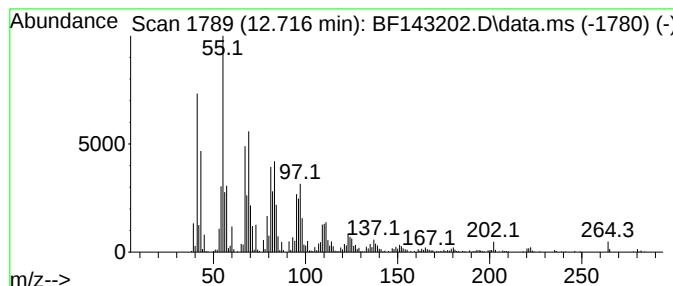
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 cis-13-Octadecenoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.716	48.04 ng	1513420	Phenanthrene-d10		11.486	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	cis-13-Octadecenoic acid		282	C18H34O2	013126-39-1	98
2	trans-13-Octadecenoic acid		282	C18H34O2	000693-71-0	97
3	cis-Vaccenic acid		282	C18H34O2	000506-17-2	97
4	9-Octadecenoic acid, (E)-		282	C18H34O2	000112-79-8	89
5	13-Tetradecenal		210	C14H26O	085896-31-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072225\
Data File : BF143202.D
Acq On : 22 Jul 2025 21:48
Operator : RC/JU
Sample : Q2649-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

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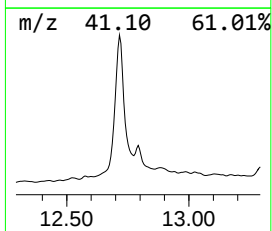
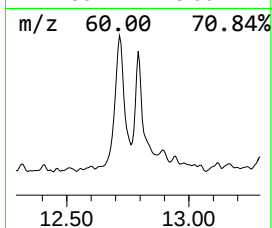
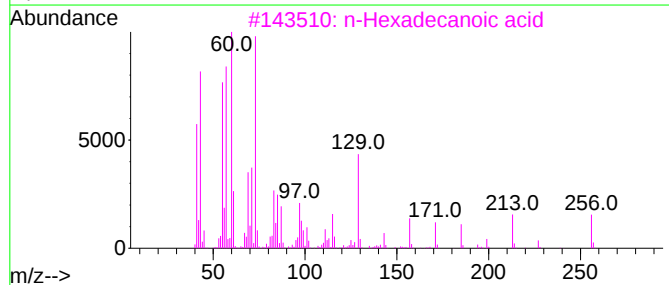
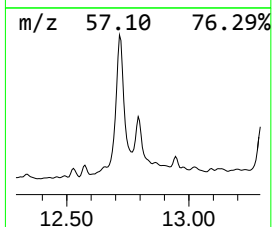
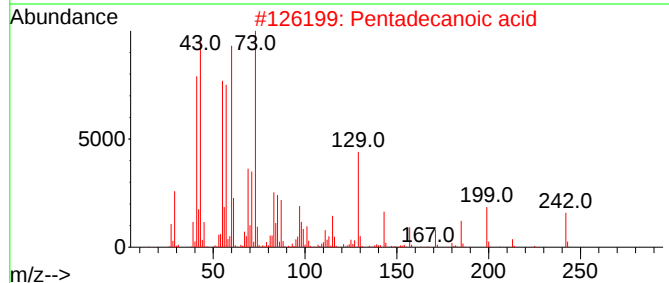
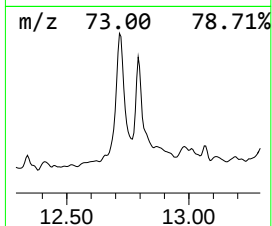
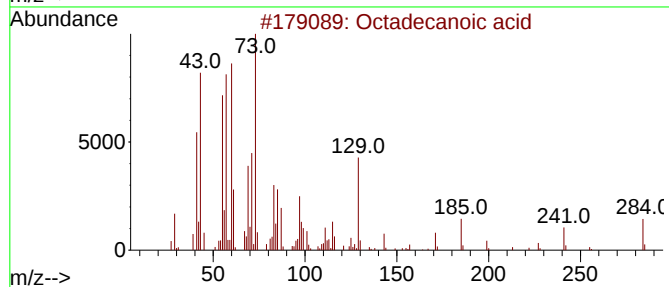
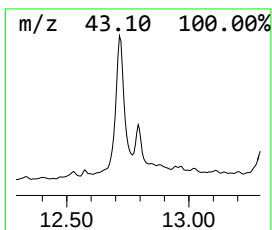
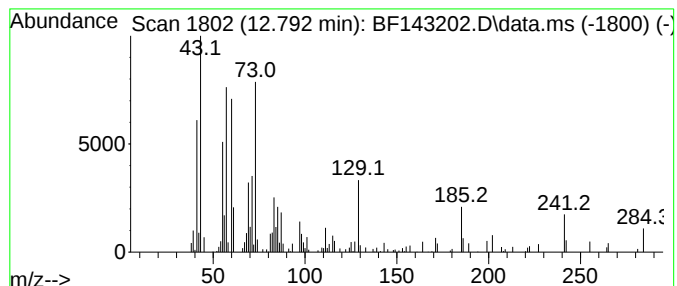
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.792	5.07 ng	159815	Phenanthrene-d10	11.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	91
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
4			Tridecanoic acid	214	C13H26O2	000638-53-9	58
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072225\
Data File : BF143202.D
Acq On : 22 Jul 2025 21:48
Operator : RC/JU
Sample : Q2649-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

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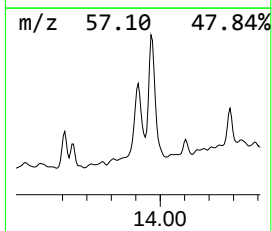
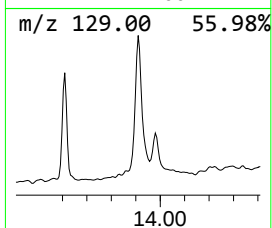
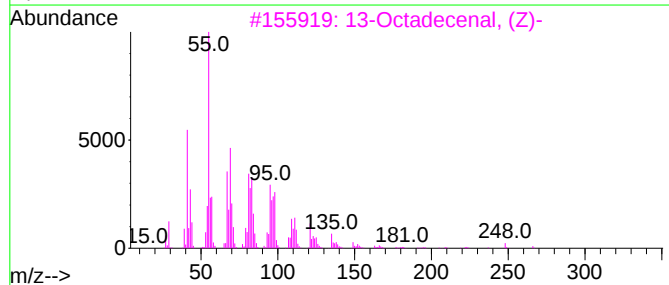
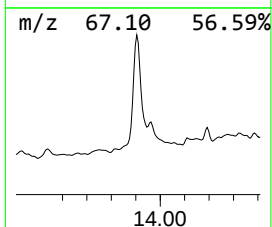
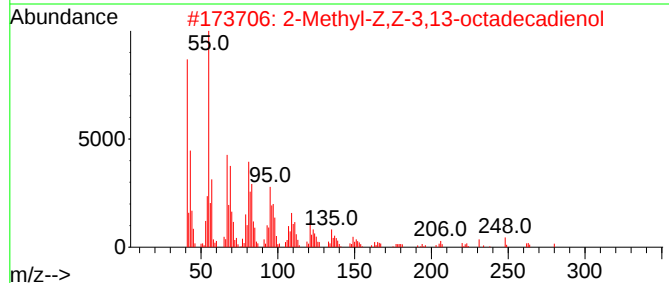
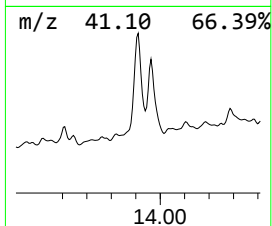
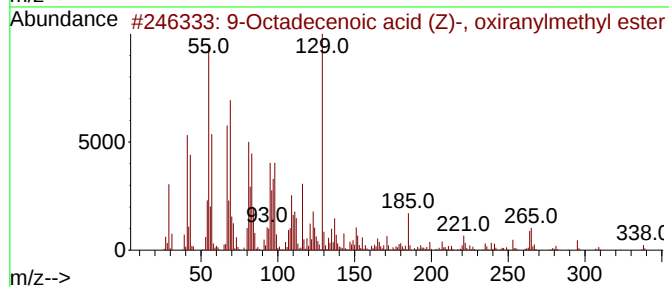
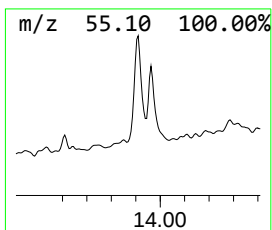
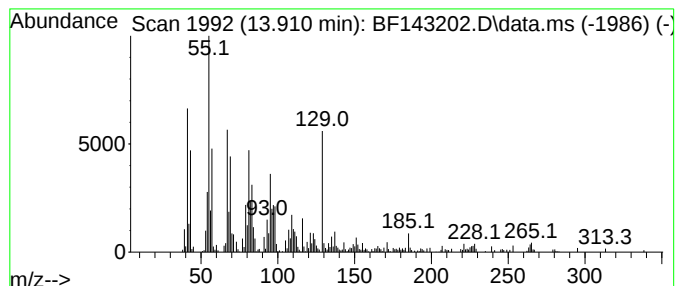
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Octadecenoic acid (Z)-, o... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	11.70 ng	413110	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid (Z)-, oxiran...	338	C21H38O3	005431-33-4	96
2			2-Methyl-Z,Z-3,13-octadecadienol	280	C19H36O	1000130-90-5	95
3			13-Octadecenal, (Z)-	266	C18H34O	058594-45-9	86
4			12-Methyl-E,E-2,13-octadecadien...	280	C19H36O	1010130-90-4	84
5			9,12-Octadecadien-1-ol, (Z,Z)-	266	C18H34O	000506-43-4	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072225\
Data File : BF143202.D
Acq On : 22 Jul 2025 21:48
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Sample : Q2649-13
Misc :
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Instrument :
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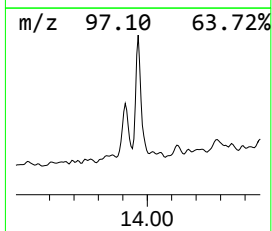
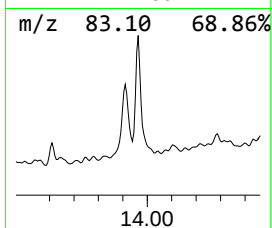
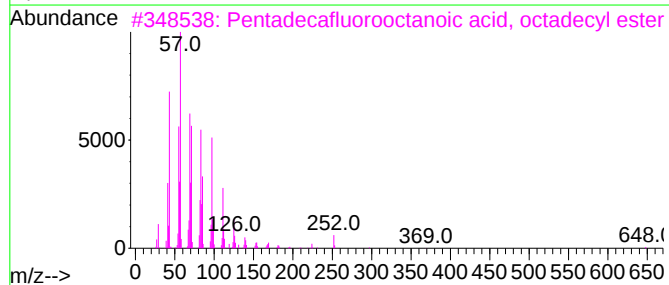
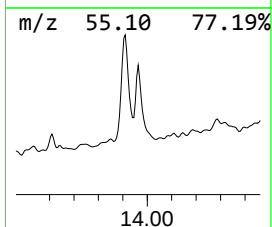
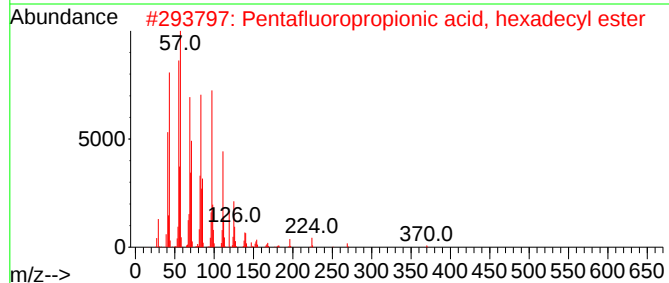
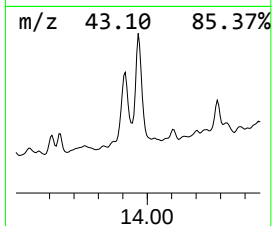
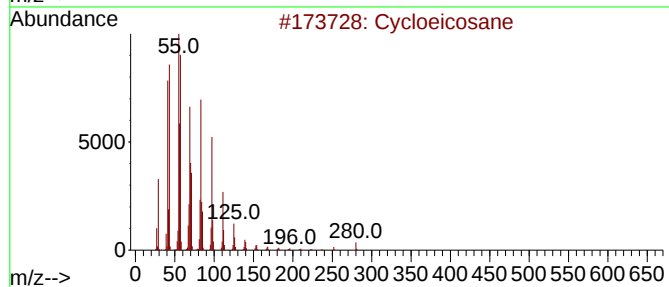
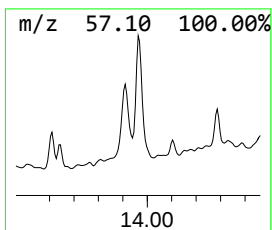
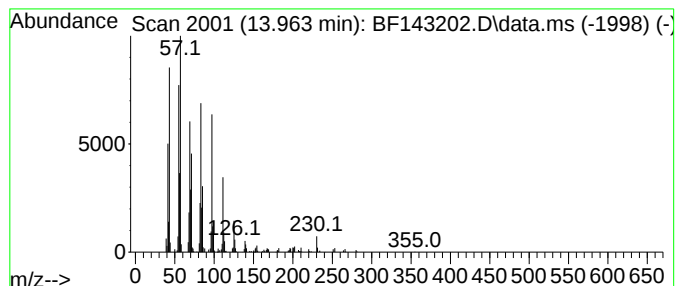
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cycloeicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.963	7.28 ng	257095	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloeicosane	280	C20H40	000296-56-0	98
2			Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	91
3			Pentadecafluorooctanoic acid, octadecyl ester	666	C26H37F15O2	1000406-04-8	91
4			Trichloroacetic acid, hexadecyl ester	386	C18H33Cl3O2	074339-54-1	91
5			Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072225\
Data File : BF143202.D
Acq On : 22 Jul 2025 21:48
Operator : RC/JU
Sample : Q2649-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

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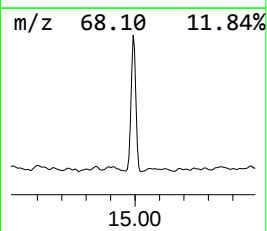
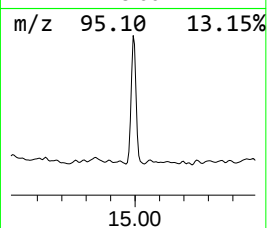
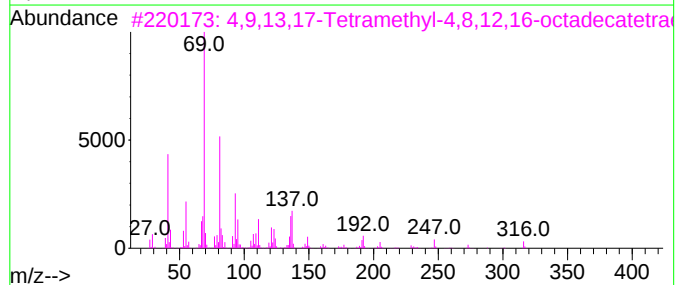
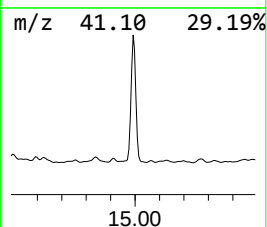
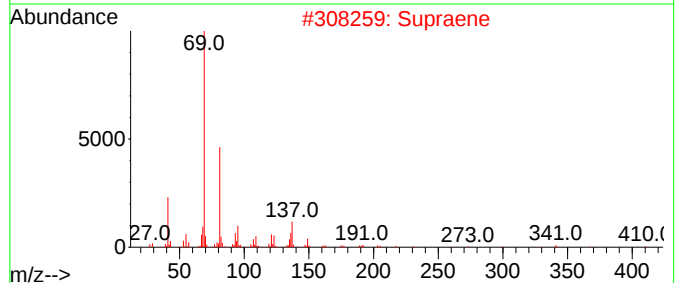
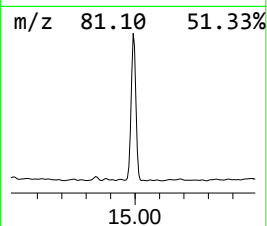
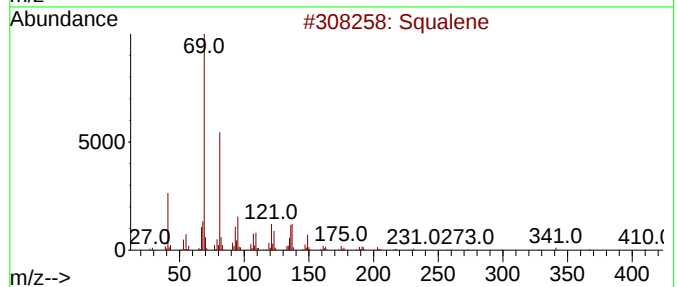
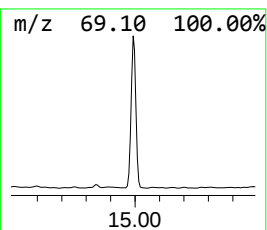
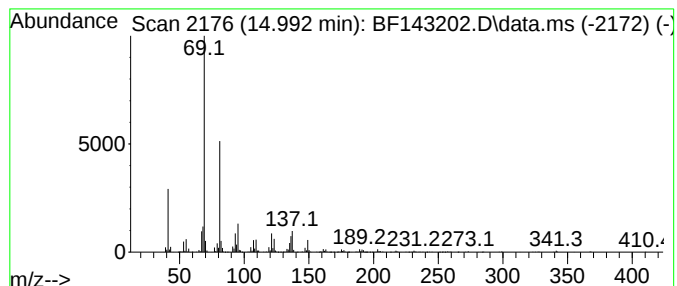
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.992	26.04 ng	664671	Perylene-d12	15.639

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	94
2			Supraene	410	C30H50	007683-64-9	91
3			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4			Trideca-1,7,11-triene-1,1-dicarb...	270	C18H26N2	1000161-46-0	53
5			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072225\
Data File : BF143202.D
Acq On : 22 Jul 2025 21:48
Operator : RC/JU
Sample : Q2649-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.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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2-Pentanone, 4-...	5.198	8.1	ng	261844	1	6.969	645953	20.0
Benzophenone	10.710	8.4	ng	302006	3	10.004	718824	20.0
Tetradecanoic acid	11.145	2.9	ng	89995	4	11.486	630108	20.0
1,9-Tetradecadiene	11.933	4.4	ng	139166	4	11.486	630108	20.0
n-Hexadecanoic ...	12.010	17.8	ng	561682	4	11.486	630108	20.0
cis-13-Octadece...	12.716	48.0	ng	1513420	4	11.486	630108	20.0
Octadecanoic acid	12.792	5.1	ng	159815	4	11.486	630108	20.0
9-Octadecenoic ...	13.910	11.7	ng	413110	5	14.127	705974	20.0
Cycloeicosane	13.963	7.3	ng	257095	5	14.127	705974	20.0
Squalene	14.992	26.0	ng	664671	6	15.639	510438	20.0