

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051625\
 Data File : BF142439.D
 Acq On : 16 May 2025 21:08
 Operator : RC/JU
 Sample : Q2043-03
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-12000

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-BF050525.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142439.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.546	384	400	411	rBV3	46916	122491	3.09%	0.539%
2	5.099	489	494	501	rVB	125511	181448	4.57%	0.798%
3	5.510	558	564	572	rBV	1134068	1550647	39.09%	6.818%
4	6.522	730	736	741	rBV	1150289	1495316	37.69%	6.575%
5	6.904	794	801	807	rBV	444528	610121	15.38%	2.683%
6	7.457	886	895	900	rBV2	706099	1101707	27.77%	4.844%
7	8.187	1012	1019	1023	rBV	506202	711492	17.93%	3.128%
8	8.363	1042	1049	1051	rBV3	92439	166321	4.19%	0.731%
9	8.398	1051	1055	1057	rVV	154552	218471	5.51%	0.961%
10	8.422	1057	1059	1064	rVB	180313	213228	5.37%	0.938%
11	8.475	1065	1068	1074	rVV4	97492	168114	4.24%	0.739%
12	8.604	1086	1090	1096	rBV	256215	478035	12.05%	2.102%
13	8.775	1115	1119	1122	rBV	278619	393093	9.91%	1.728%
14	8.869	1133	1135	1139	rVB2	199385	215737	5.44%	0.949%
15	9.063	1165	1168	1171	rBV4	228984	366969	9.25%	1.613%
16	9.210	1189	1193	1197	rVB	1011992	1284555	32.38%	5.648%
17	9.257	1197	1201	1205	rBV	1267099	1622488	40.90%	7.134%
18	9.345	1212	1216	1220	rBV3	1261186	2132773	53.76%	9.377%
19	9.669	1266	1271	1274	rBV3	2070483	3967296	100.00%	17.443%
20	9.863	1301	1304	1308	rBV2	1517968	2053789	51.77%	9.030%
21	16.780	2475	2480	2494	rVB	1602466	3690004	93.01%	16.224%

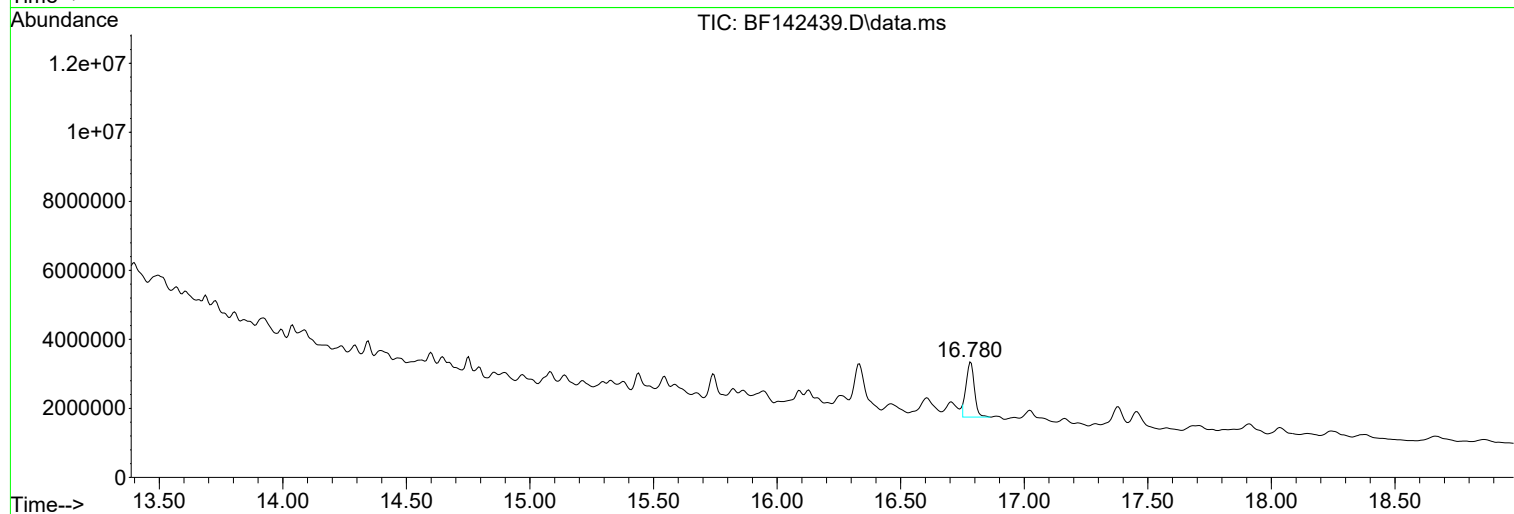
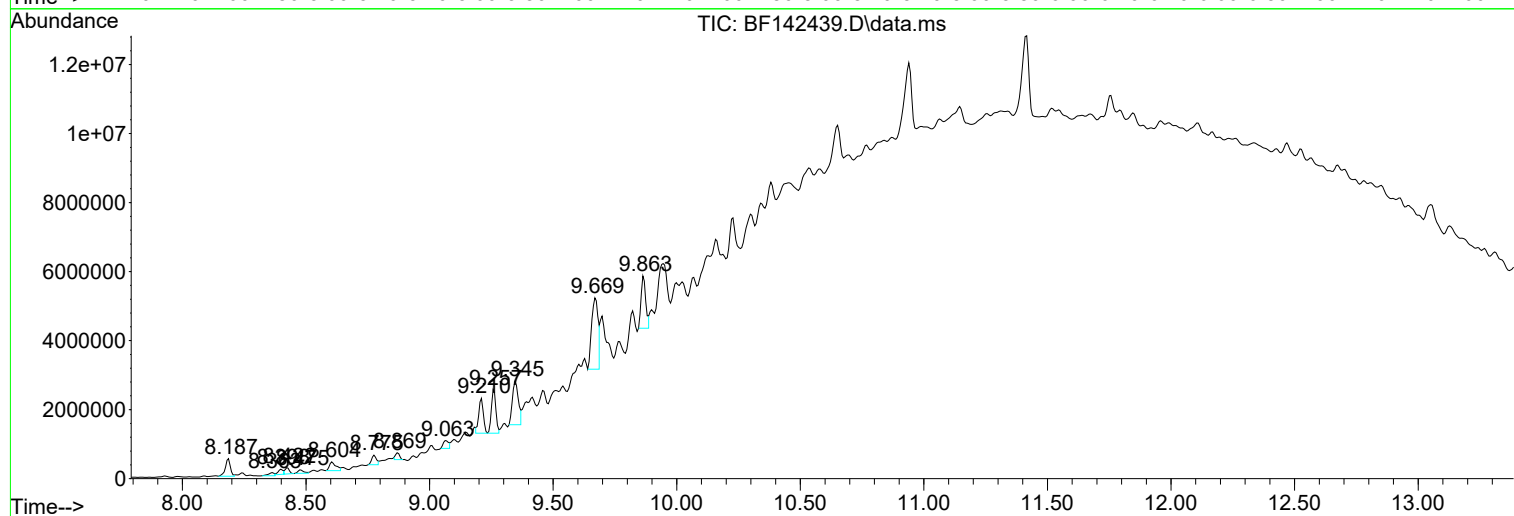
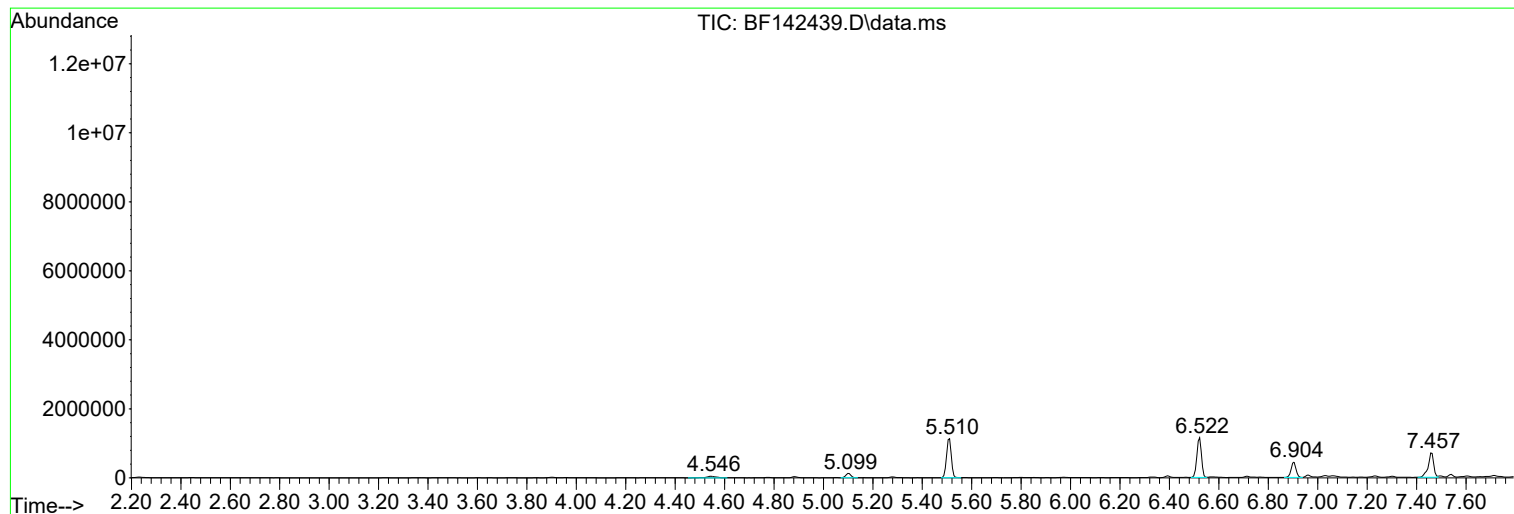
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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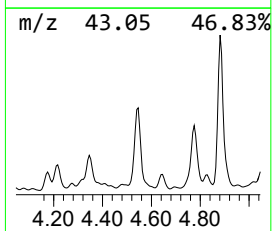
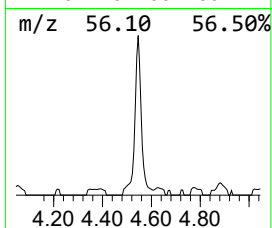
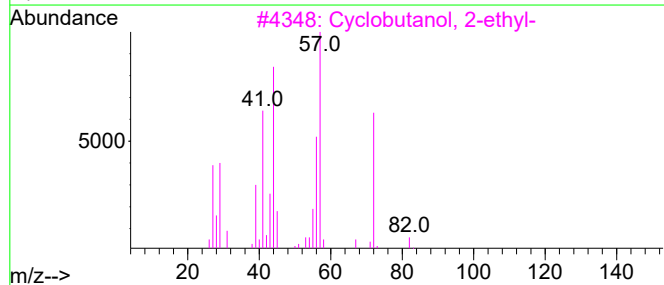
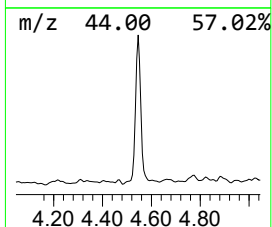
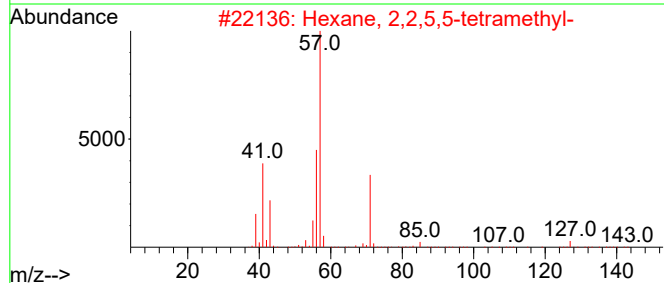
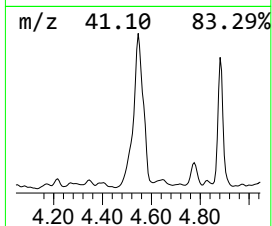
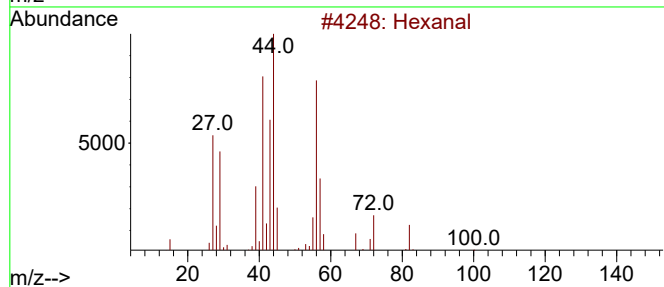
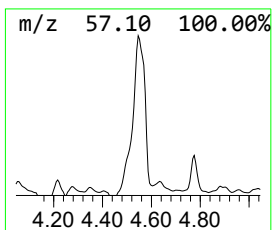
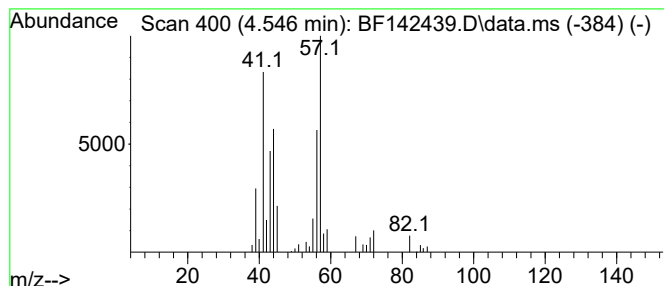
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexanal Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.546	4.02 ng	122491	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	53
2			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	38
3			Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	37
4			Oxirane, 2-methyl-3-(1-methyleth...	100	C6H12O	001192-31-0	37
5			n-Hexane	86	C6H14	000110-54-3	35



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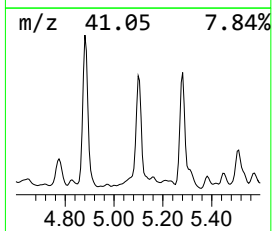
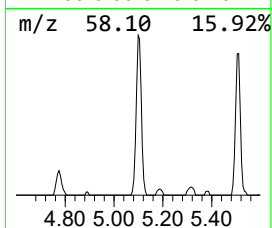
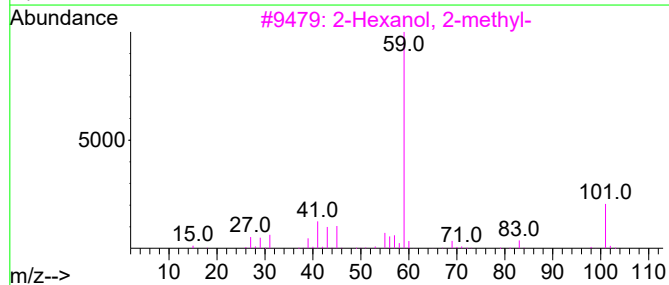
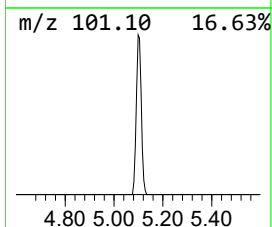
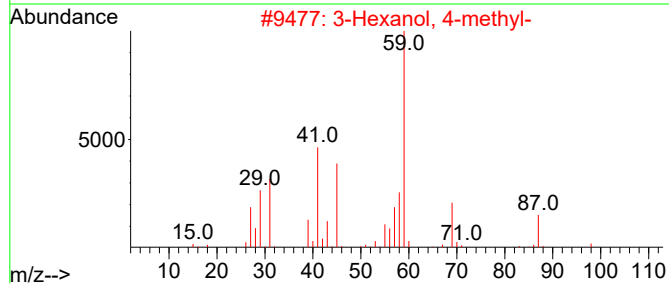
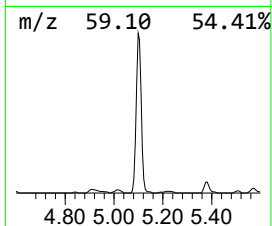
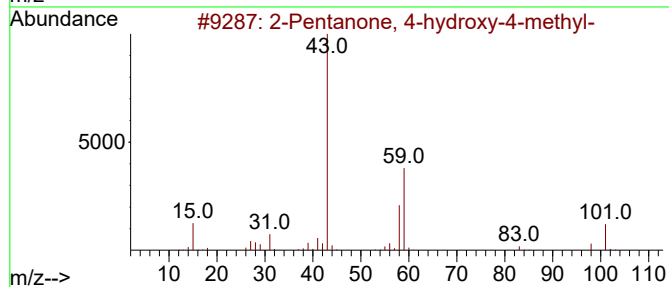
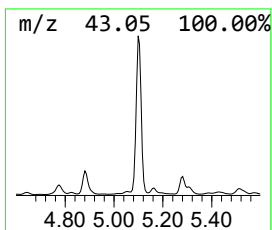
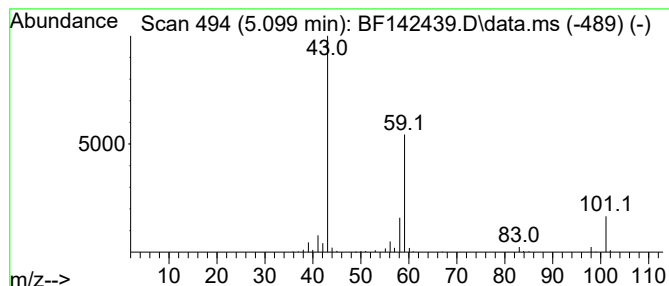
Instrument :
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ClientSampleId :
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.099	5.95 ng	181448	1,4-Dichlorobenzene-d4			6.904
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	16



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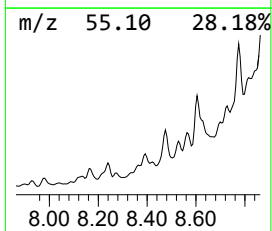
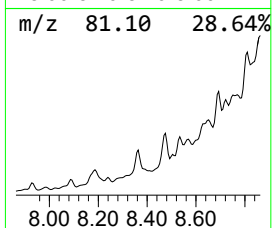
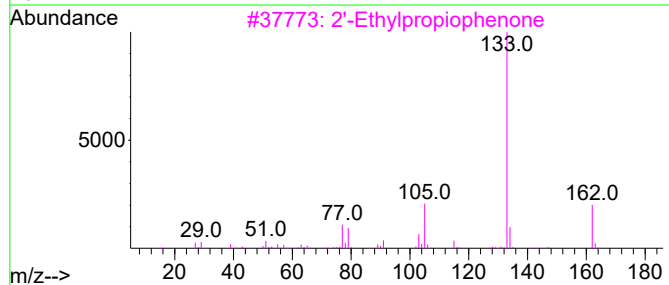
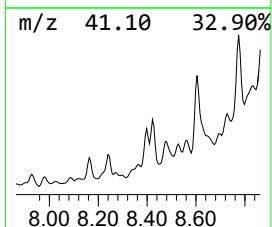
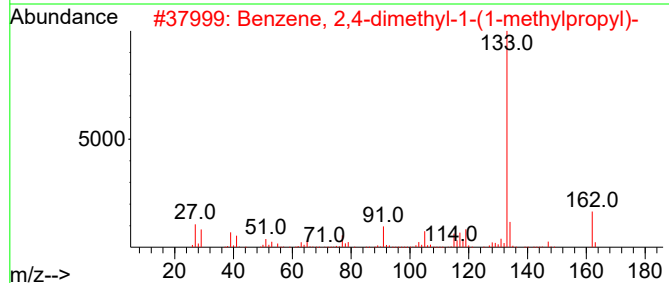
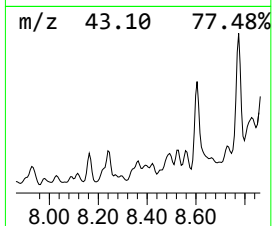
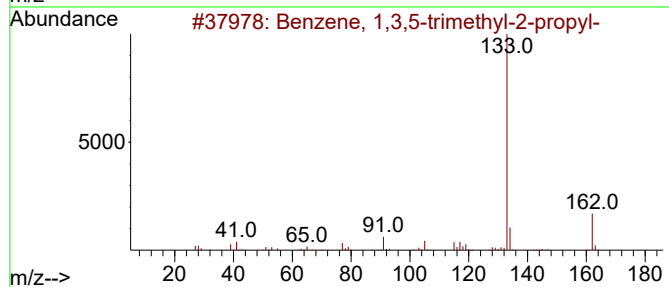
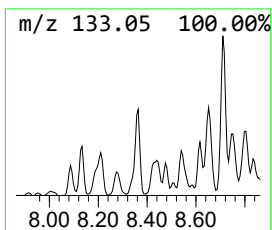
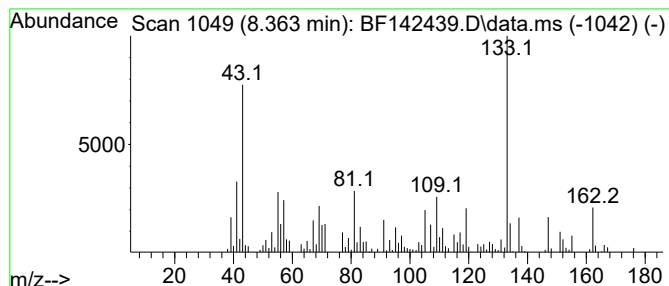
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Peak Number 3 Benzene, 1,3,5-trimethyl-2-... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.363	4.68 ng	166321	Naphthalene-d8	8.187

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3,5-trimethyl-2-propyl-	162	C12H18	004810-04-2	60
2			Benzene, 2,4-dimethyl-1-(1-methy...	162	C12H18	001483-60-9	60
3			2'-Ethylpropiophenone	162	C11H14O	016819-79-7	49
4			Benzene, 1-ethyl-3-(1-methylethyl)-	148	C11H16	004920-99-4	49
5			Phenol, 4-cyclopentyl-	162	C11H14O	001518-83-8	43



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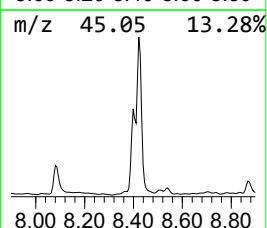
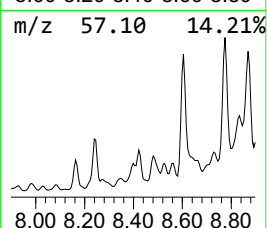
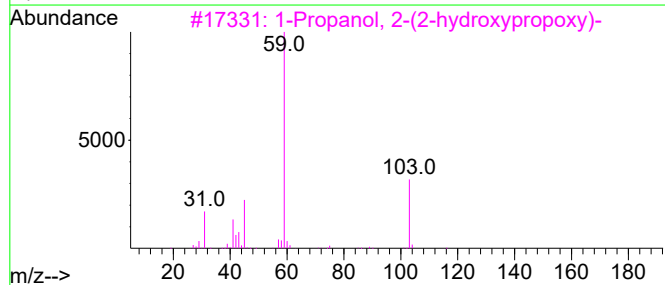
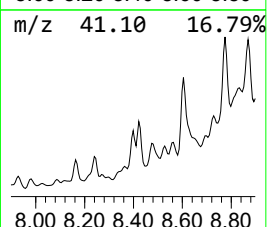
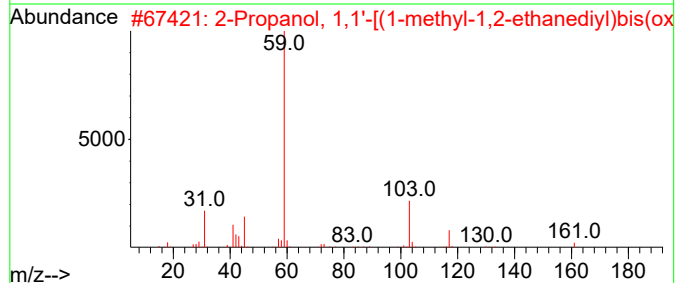
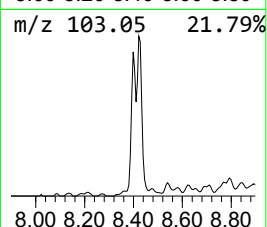
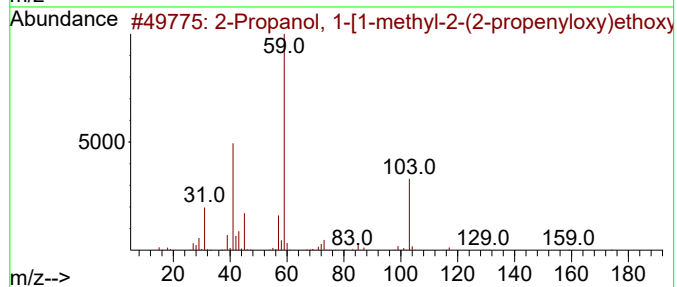
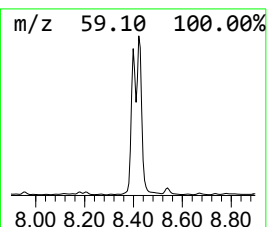
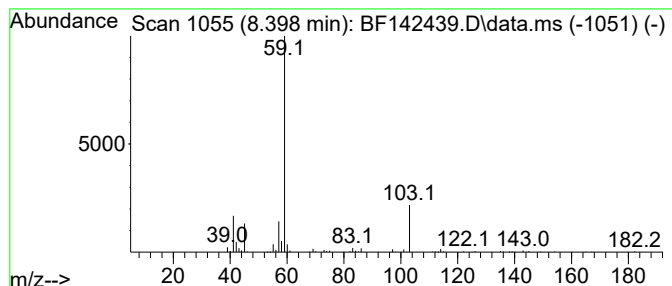
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Peak Number 4 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.398	6.14 ng	218471	Naphthalene-d8	8.187

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	78	
2	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	78	
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78	
4	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	72	
5	1-(1-tert-Butoxypropan-2-yloxy)p...	190	C10H22O3	132739-31-2	64	



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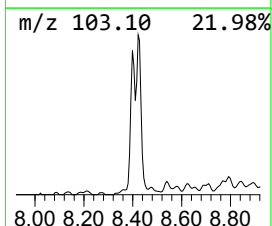
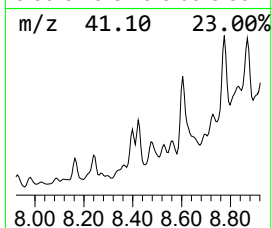
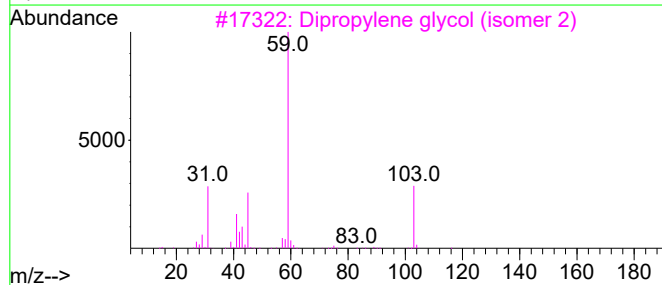
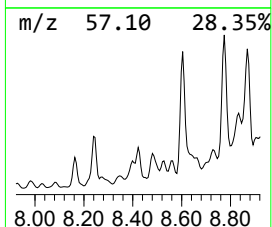
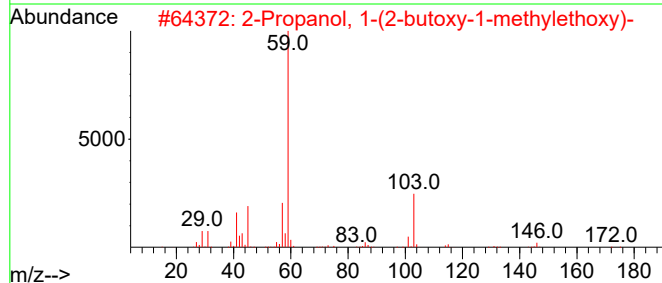
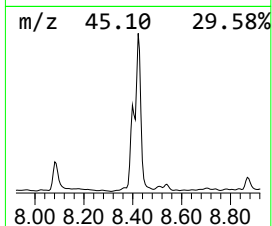
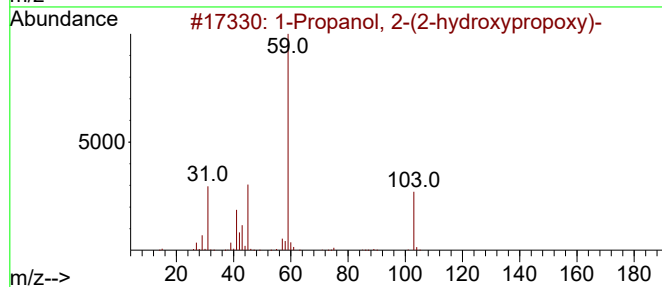
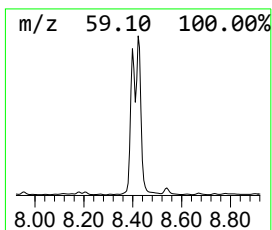
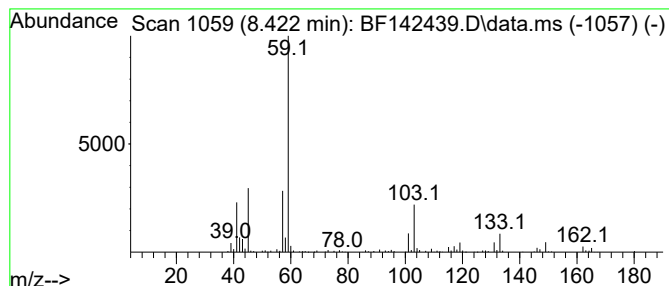
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Peak Number 5 1-Propanol, 2-(2-hydroxypro... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.422	5.99 ng	213228	Naphthalene-d8	8.187

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64		
2	2-Propanol, 1-(2-butoxy-1-methyl...)	190	C10H22O3	029911-28-2	59		
3	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	53		
4	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	53		
5	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	53		



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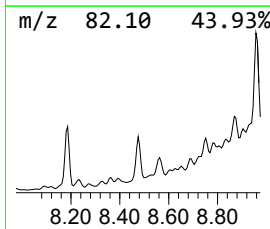
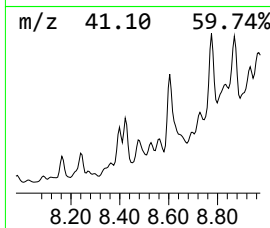
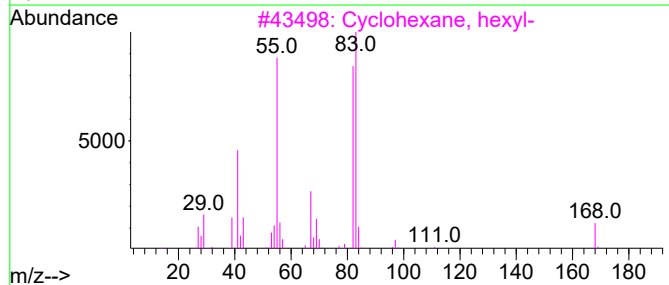
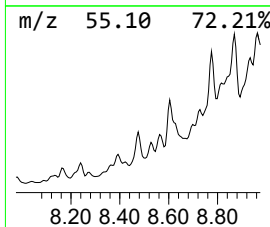
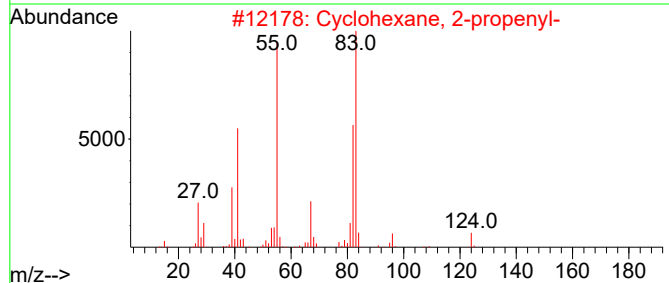
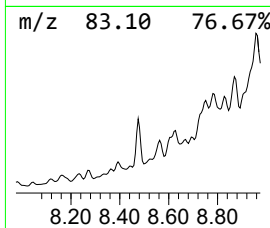
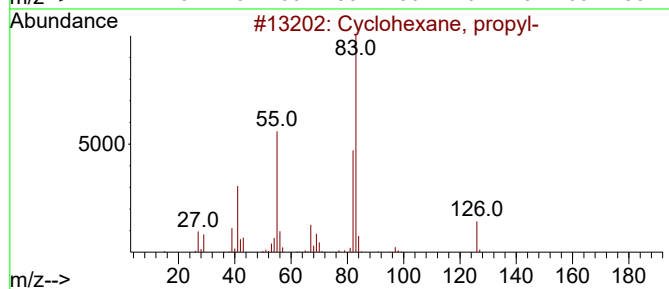
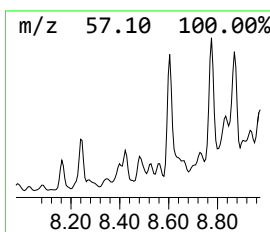
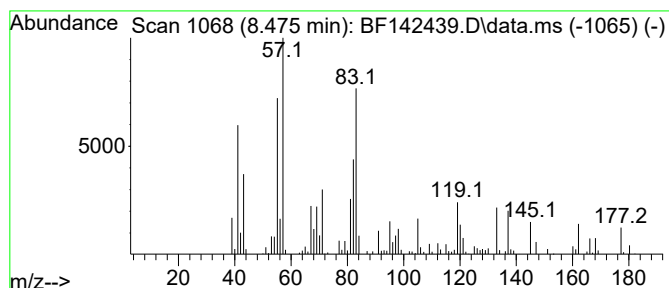
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown8.475 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.475	4.73 ng	168114	Naphthalene-d8	8.187

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, propyl-	126	C9H18	001678-92-8	43
2			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	38
3			Cyclohexane, hexyl-	168	C12H24	004292-75-5	38
4			Cyclohexane, ethyl-	112	C8H16	001678-91-7	38
5			1-Cyclohexylethanol, pentafluoro...	274	C11H15F5O2	1000365-50-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051625\
Data File : BF142439.D
Acq On : 16 May 2025 21:08
Operator : RC/JU
Sample : Q2043-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12000

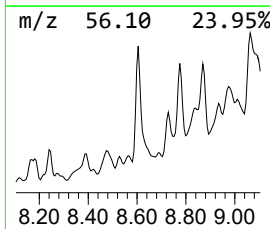
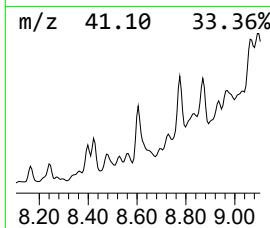
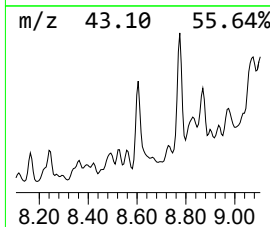
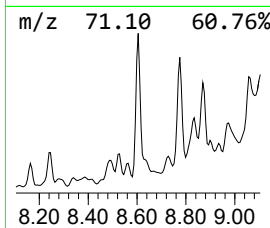
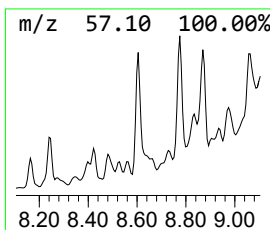
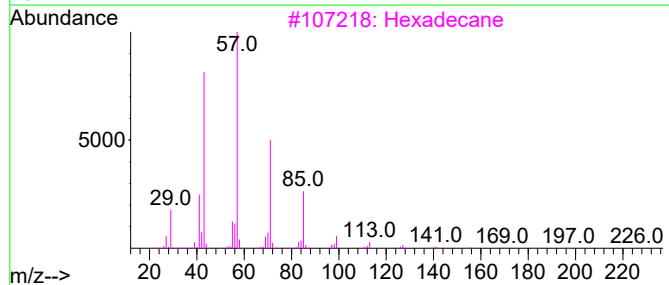
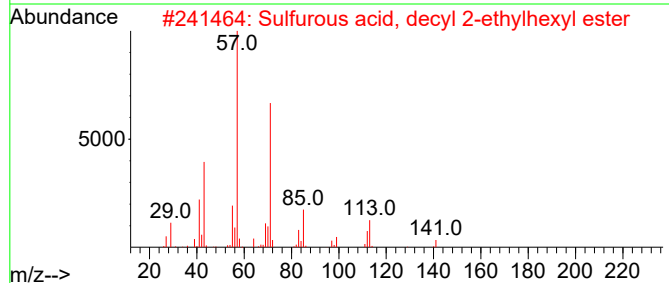
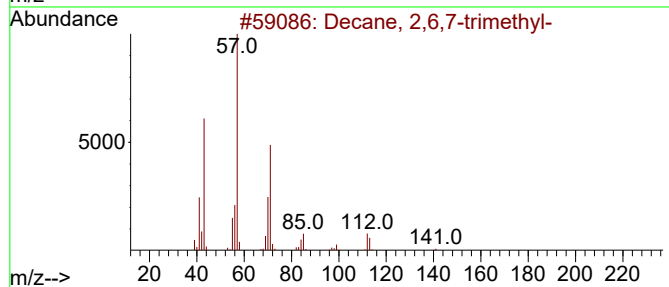
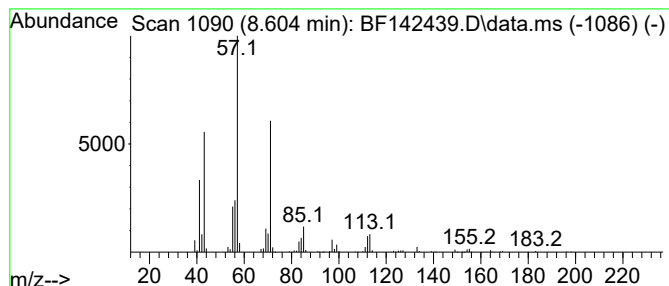
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Decane, 2,6,7-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.604	13.44 ng	478035	Naphthalene-d8	8.187

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	90
2			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	59
3			Hexadecane	226	C16H34	000544-76-3	59
4			Nonane, 3-methyl-	142	C10H22	005911-04-6	59
5			Tridecane, 3-methyl-	198	C14H30	006418-41-3	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051625\
Data File : BF142439.D
Acq On : 16 May 2025 21:08
Operator : RC/JU
Sample : Q2043-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12000

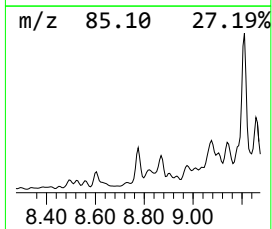
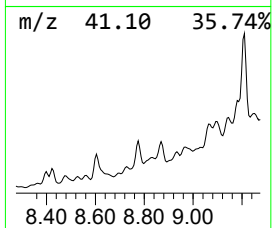
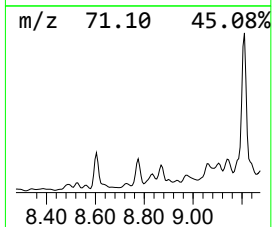
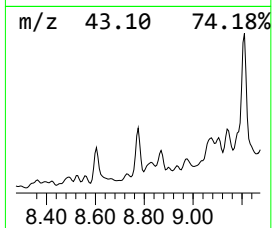
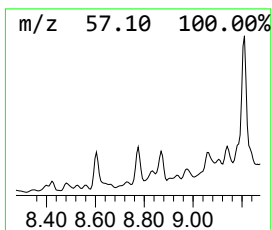
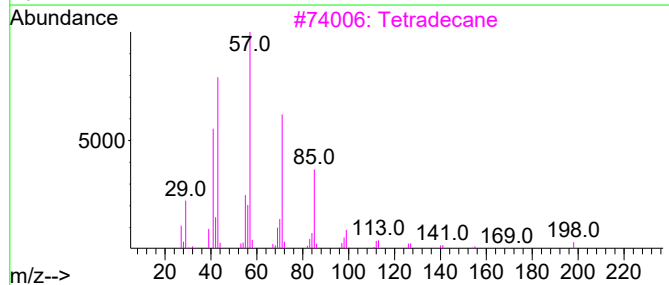
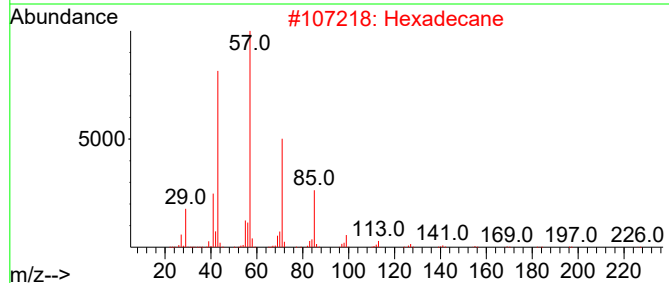
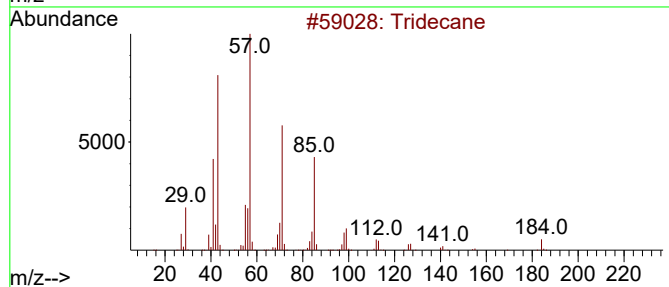
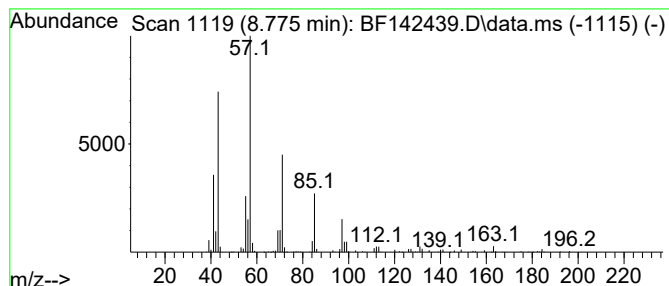
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.775	11.05 ng	393093	Naphthalene-d8	8.187

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	94
2			Hexadecane	226	C16H34	000544-76-3	80
3			Tetradecane	198	C14H30	000629-59-4	72
4			Dodecane	170	C12H26	000112-40-3	72
5			Undecane	156	C11H24	001120-21-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051625\
Data File : BF142439.D
Acq On : 16 May 2025 21:08
Operator : RC/JU
Sample : Q2043-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

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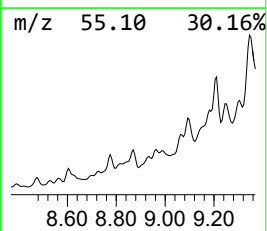
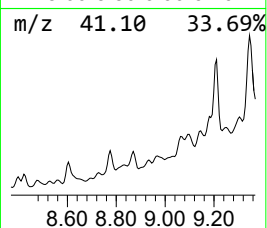
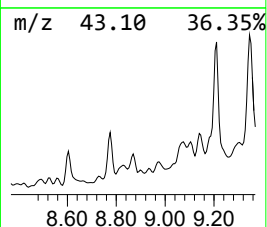
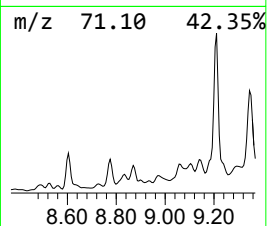
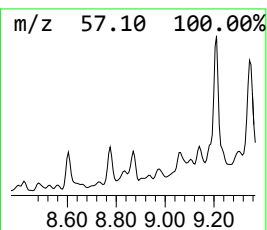
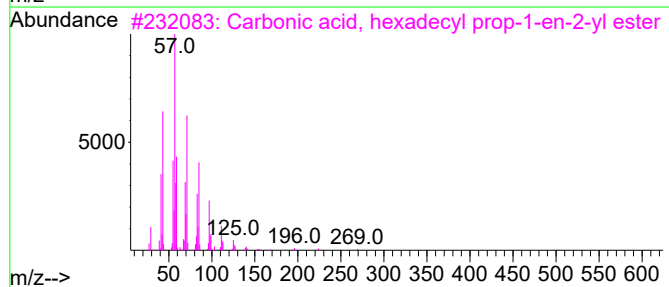
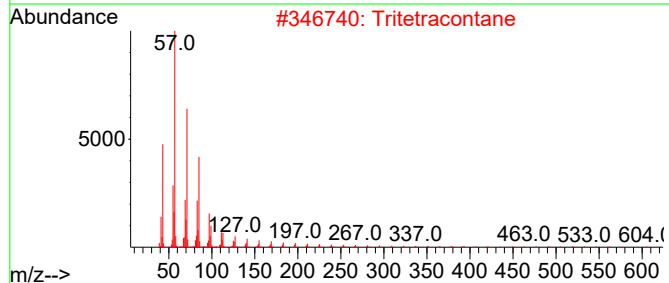
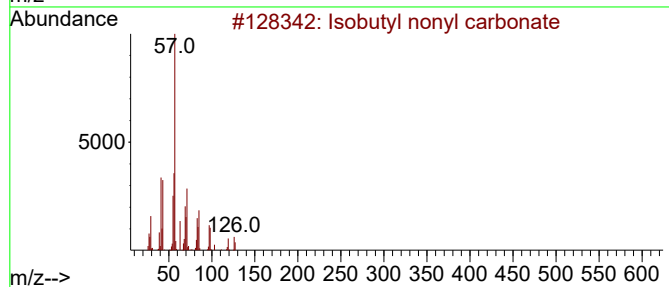
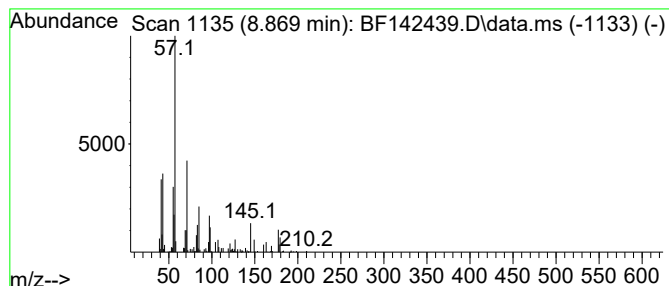
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Isobutyl nonyl carbonate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.869	6.06 ng	215737	Naphthalene-d8	8.187

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutyl nonyl carbonate	244	C14H28O3	959311-27-4	59
2			Tritetracontane	605	C43H88	007098-21-7	50
3			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	50
4			Dodecane, 2,5-dimethyl-	198	C14H30	056292-65-0	50
5			Tridecane, 6-methyl-	198	C14H30	013287-21-3	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051625\
Data File : BF142439.D
Acq On : 16 May 2025 21:08
Operator : RC/JU
Sample : Q2043-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

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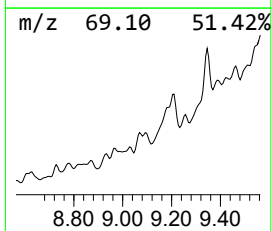
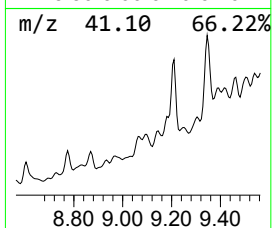
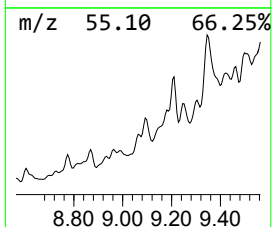
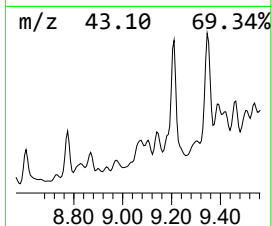
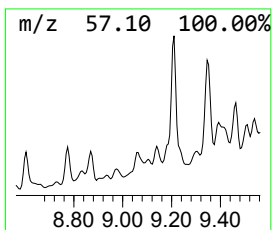
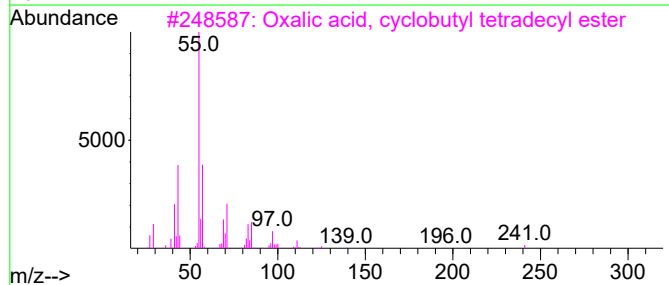
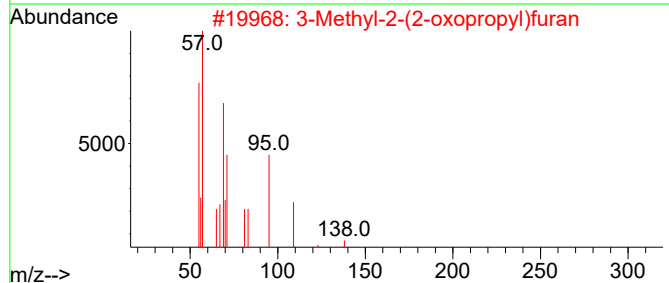
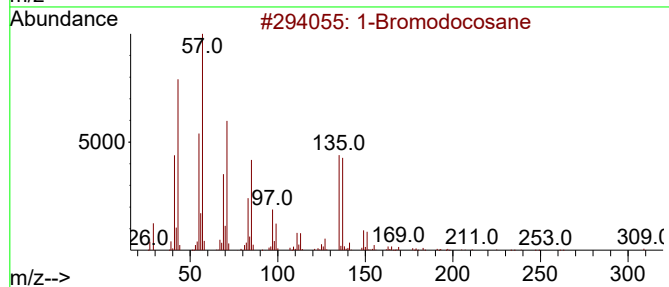
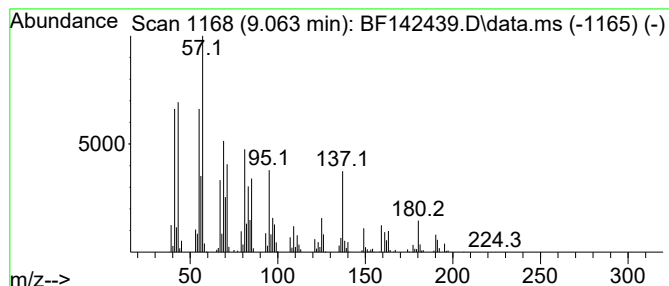
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown9.063 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.063	10.32 ng	366969	Naphthalene-d8	8.187

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Bromodocosane	388	C22H45Br	006938-66-5	43
2		3-Methyl-2-(2-oxopropyl)furan	138	C8H10O2	087773-62-4	38
3		Oxalic acid, cyclobutyl tetradec...	340	C20H36O4	1000309-70-9	30
4		Nonyl tetradecyl ether	340	C23H48O	1000406-37-6	27
5		Decane, 5-cyclohexyl-	224	C16H32	013151-76-3	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051625\
Data File : BF142439.D
Acq On : 16 May 2025 21:08
Operator : RC/JU
Sample : Q2043-03
Misc :
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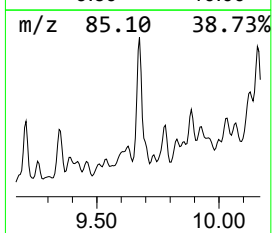
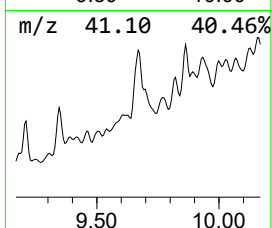
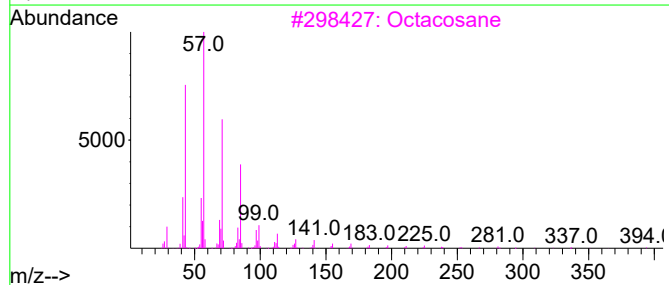
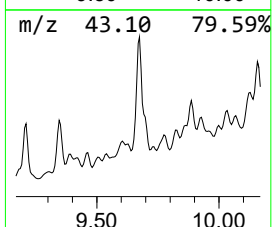
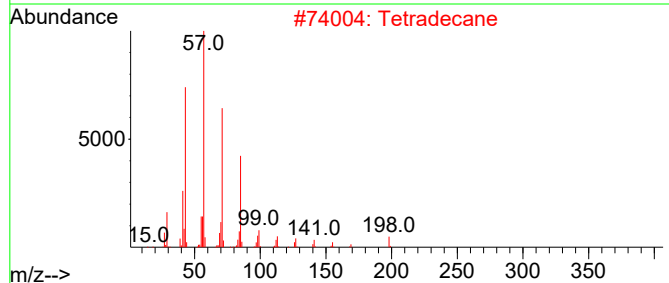
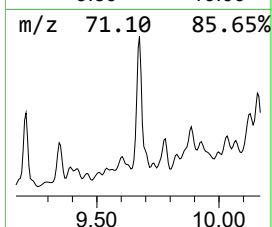
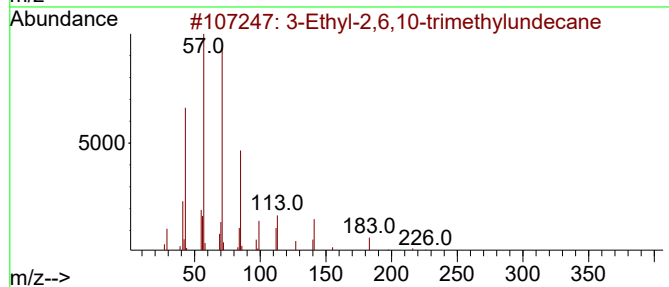
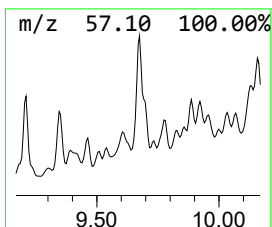
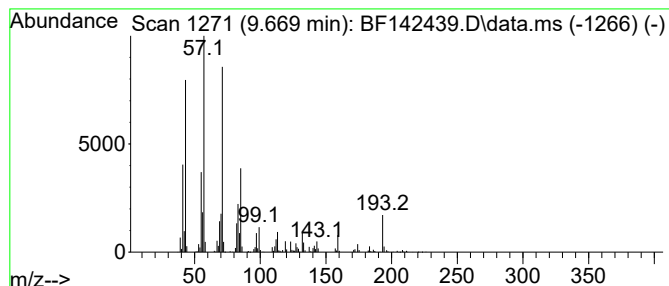
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 3-Ethyl-2,6,10-trimethylund... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
9.669	38.63 ng	3967300	Acenaphthene-d10			9.951
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3-Ethyl-2,6,10-trimethylundecane		226	C16H34	1000432-25-9	76
2	Tetradecane		198	C14H30	000629-59-4	76
3	Octacosane		394	C28H58	000630-02-4	74
4	Dodecane, 4-methyl-		184	C13H28	006117-97-1	70
5	Tridecane, 5-propyl-		226	C16H34	055045-11-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051625\
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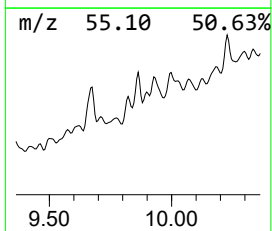
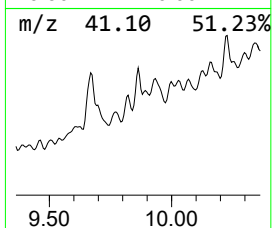
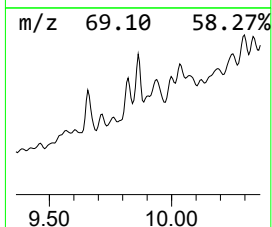
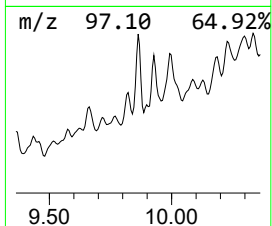
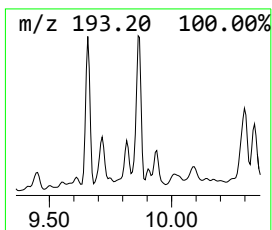
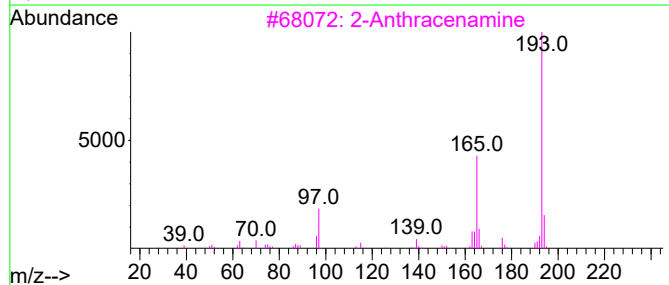
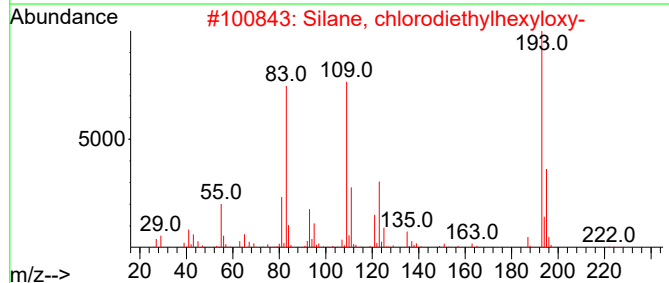
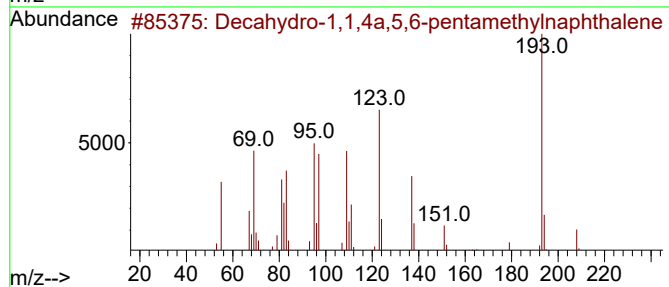
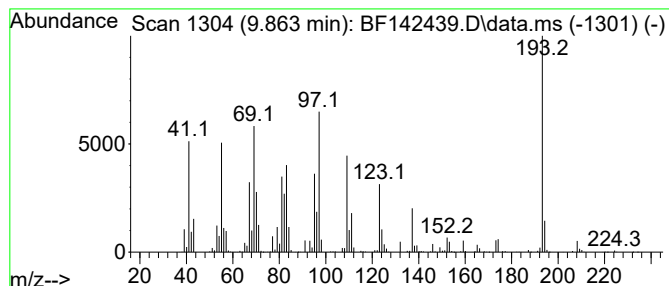
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown9.863 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.863	20.00 ng	2053790	Acenaphthene-d10	9.951	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	47
2	Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	40
3	2-Anthracenamine	193	C14H11N	000613-13-8	35
4	2-Phenylindolizine	193	C14H11N	025379-20-8	32
5	Acetylene, 1-(2-aminophenyl)-2-p...	193	C14H11N	1000380-73-4	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051625\
Data File : BF142439.D
Acq On : 16 May 2025 21:08
Operator : RC/JU
Sample : Q2043-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

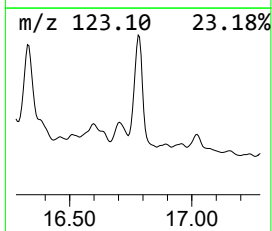
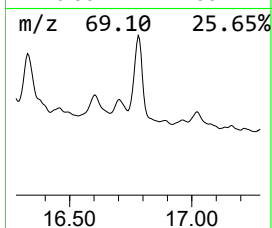
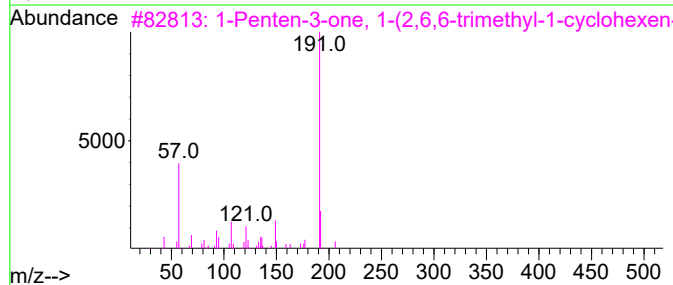
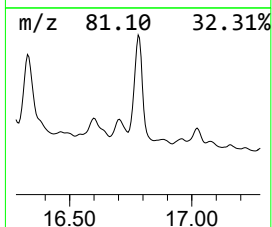
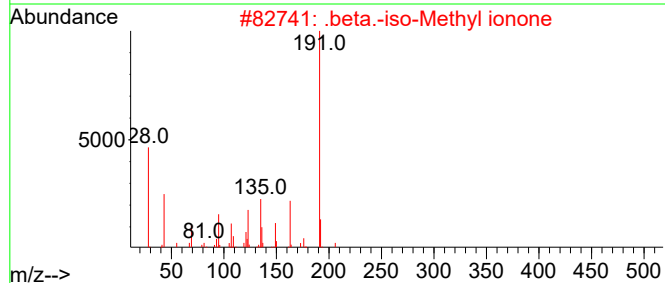
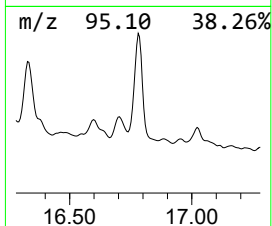
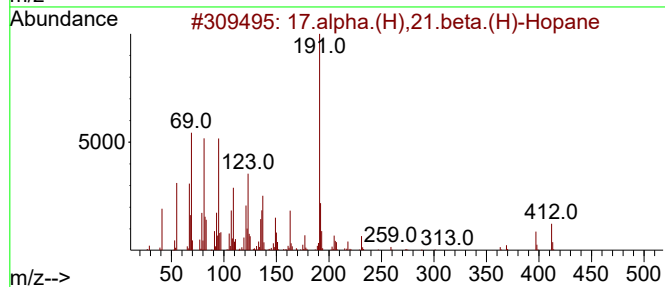
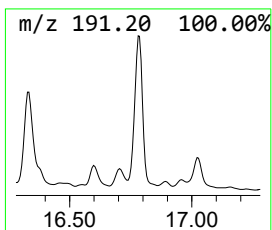
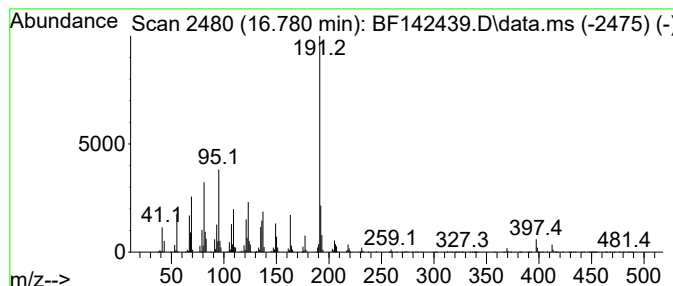
Instrument :
BNA_F
ClientSampleId :
72-12000

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 17.alpha.(H),21.beta.(H)-Ho... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.780	20.00 ng	3690000	Perylene-d12		15.580	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	17.alpha.(H),21.beta.(H)-Hopane		412	C30H52	013849-96-2	94
2	.beta.-iso-Methyl ionone		206	C14H22O	1000285-40-2	60
3	1-Penten-3-one, 1-(2,6,6-trimeth...		206	C14H22O	000127-43-5	49
4	1-Cyclohexene, 1,3,3-trimethyl-2...		206	C14H22O	1000197-08-4	47
5	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...		206	C14H22O	1000195-40-9	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051625\
Data File : BF142439.D
Acq On : 16 May 2025 21:08
Operator : RC/JU
Sample : Q2043-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12000

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.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
Hexanal	4.546	4.0	ng	122491	1	6.904	610121	20.0
2-Pentanone, 4-...	5.099	6.0	ng	181448	1	6.904	610121	20.0
Benzene, 1,3,5-...	8.363	4.7	ng	166321	2	8.187	711492	20.0
2-Propanol, 1-[...	8.398	6.1	ng	218471	2	8.187	711492	20.0
1-Propanol, 2-(...	8.422	6.0	ng	213228	2	8.187	711492	20.0
unknown8.475	8.475	4.7	ng	168114	2	8.187	711492	20.0
Decane, 2,6,7-t...	8.604	13.4	ng	478035	2	8.187	711492	20.0
Tridecane	8.775	11.1	ng	393093	2	8.187	711492	20.0
Isobutyl nonyl ...	8.869	6.1	ng	215737	2	8.187	711492	20.0
unknown9.063	9.063	10.3	ng	366969	2	8.187	711492	20.0
3-Ethyl-2,6,10-...	9.669	38.6	ng	3967300	3	9.951	2053790	20.0
unknown9.863	9.863	20.0	ng	2053790	3	9.951	2053790	20.0
17.alpha.(H),21...	16.780	20.0	ng	3690000	6	15.580	3690000	20.0