

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071023\
 Data File : BF134196.D
 Acq On : 10 Jul 2023 20:37
 Operator : CG\JU
 Sample : 03514-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CP-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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134196.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	17	rVB	1170099	1532056	85.22%	9.856%
2	5.081	506	509	519	rBV	96798	112203	6.24%	0.722%
3	5.481	573	577	596	rBV	1883498	1784317	99.26%	11.479%
4	6.481	743	747	750	rBV	1897086	1678850	93.39%	10.800%
5	6.845	805	809	818	rBV	697255	608955	33.87%	3.917%
6	7.404	900	904	914	rBV	1269244	1125503	62.61%	7.241%
7	8.122	1022	1026	1039	rBV	952918	749335	41.68%	4.821%
8	9.198	1205	1209	1212	rBV	2287293	1797669	100.00%	11.565%
9	9.881	1321	1325	1332	rBV	894052	694047	38.61%	4.465%
10	10.598	1444	1447	1452	rBV	141726	123110	6.85%	0.792%
11	10.675	1456	1460	1469	rBV	1109404	1008731	56.11%	6.489%
12	11.375	1575	1579	1588	rBV	836910	721759	40.15%	4.643%
13	11.904	1666	1669	1673	rBV2	63651	71371	3.97%	0.459%
14	12.969	1846	1850	1854	rBV	1800679	1749726	97.33%	11.256%
15	13.886	2002	2006	2013	rBV3	106790	186599	10.38%	1.200%
16	14.033	2028	2031	2036	rBV	681952	675241	37.56%	4.344%
17	14.198	2057	2059	2064	rVB2	41118	51132	2.84%	0.329%
18	14.463	2101	2104	2108	rBV4	48455	82418	4.58%	0.530%
19	14.804	2159	2162	2172	rBV	132482	191834	10.67%	1.234%
20	14.898	2175	2178	2182	rVB	63918	66623	3.71%	0.429%
21	15.539	2283	2287	2296	rVB	384841	533021	29.65%	3.429%

Sum of corrected areas: 15544500

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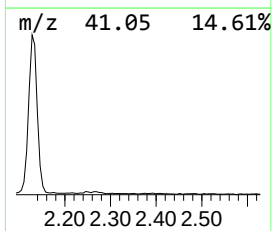
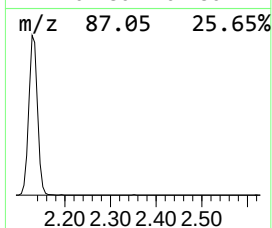
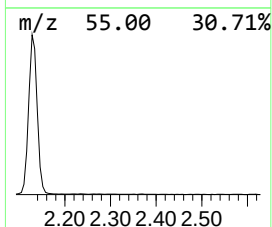
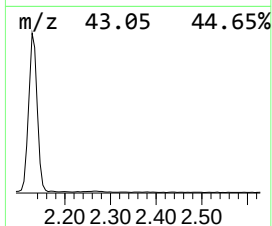
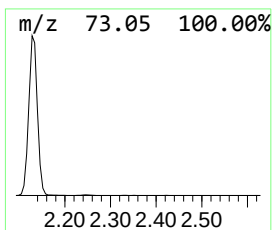
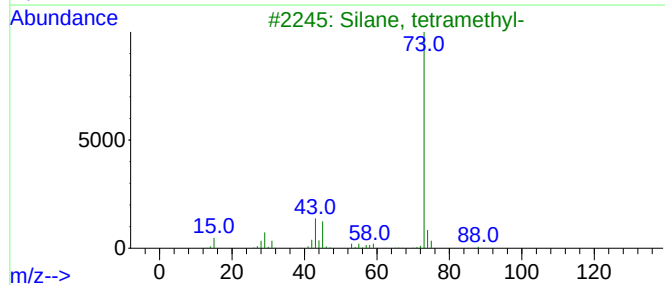
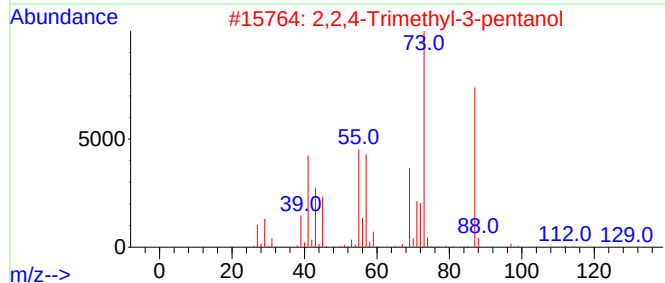
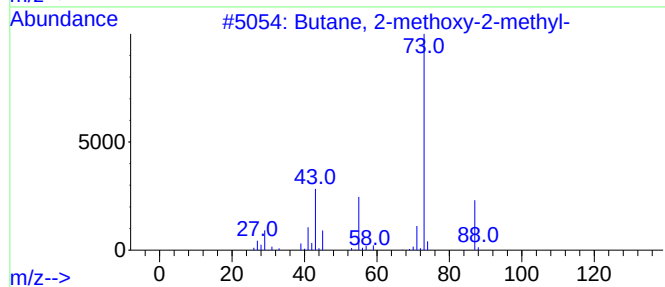
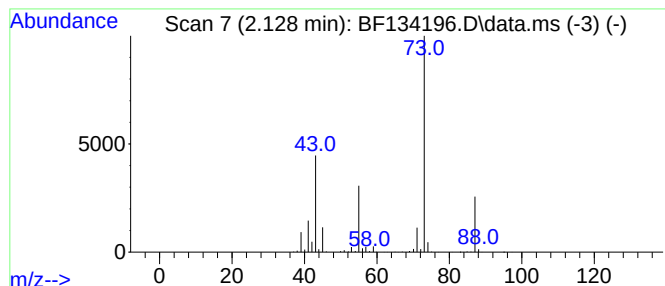
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	50.32 ng	1532060	1,4-Dichlorobenzene-d4	6.845

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	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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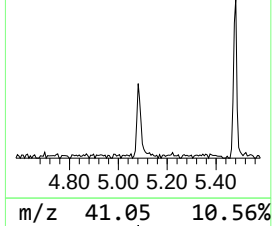
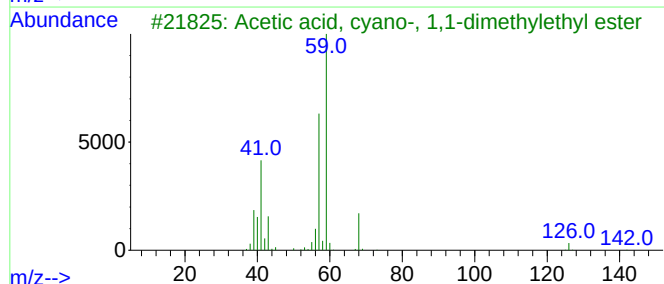
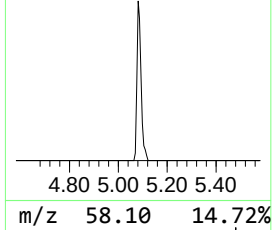
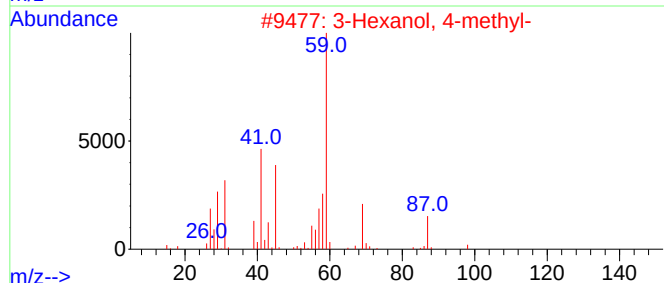
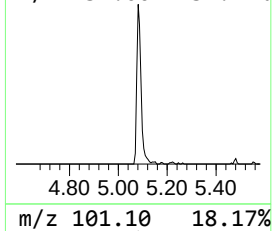
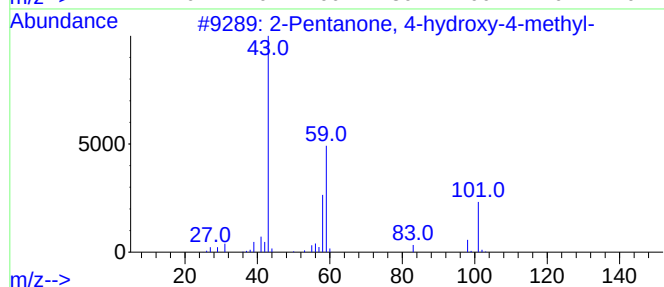
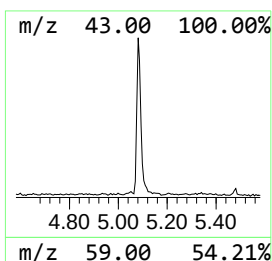
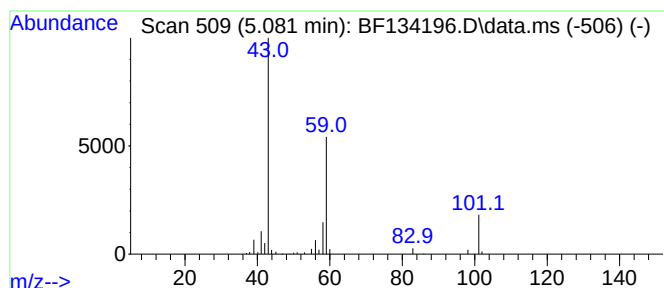
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	3.69 ng	112203	1,4-Dichlorobenzene-d4	6.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9



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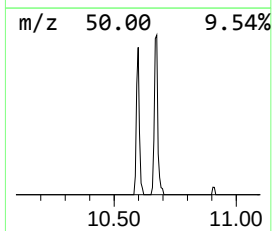
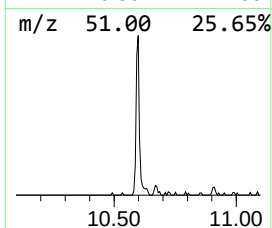
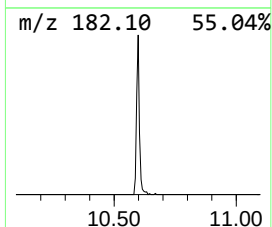
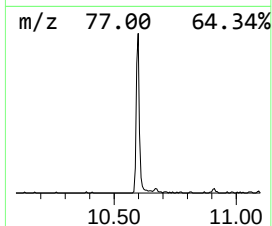
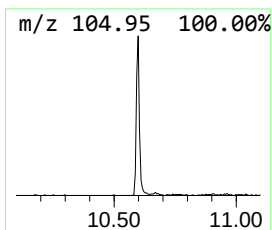
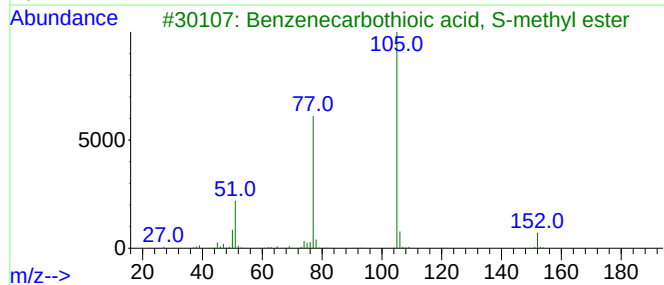
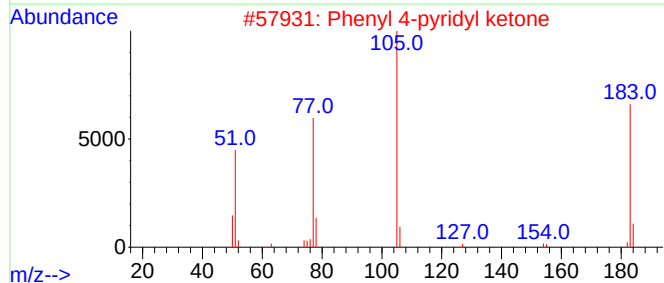
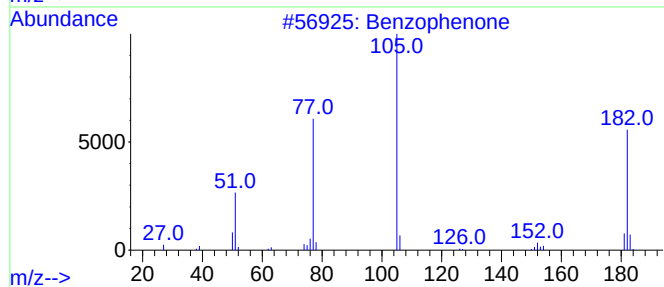
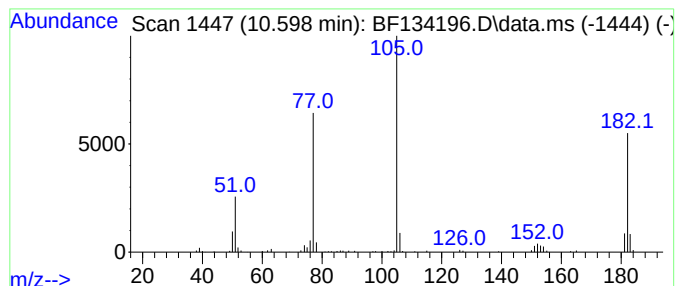
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.598	3.55 ng	123110	Acenaphthene-d10	9.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	52
5			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	52



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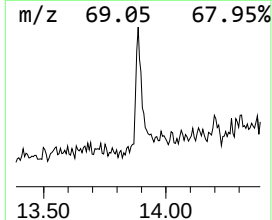
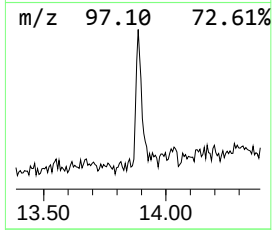
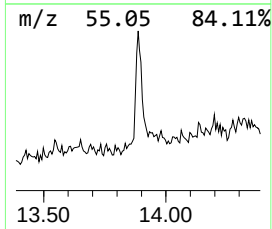
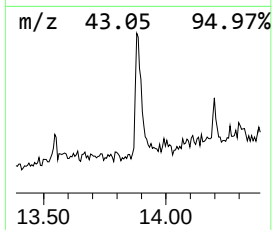
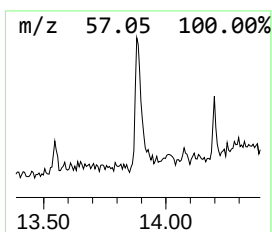
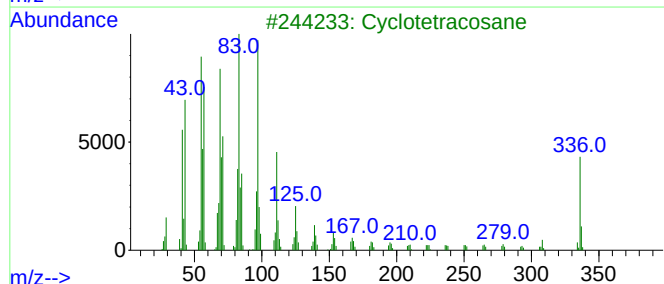
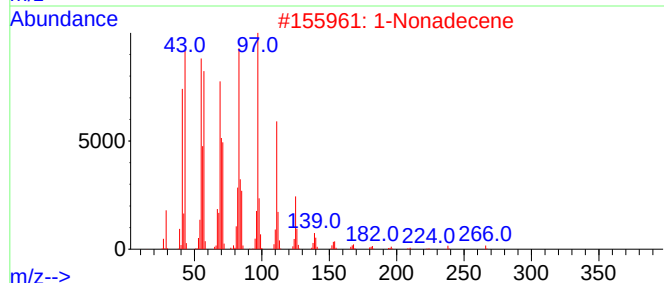
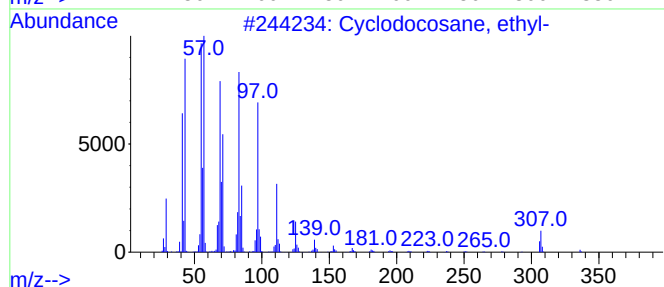
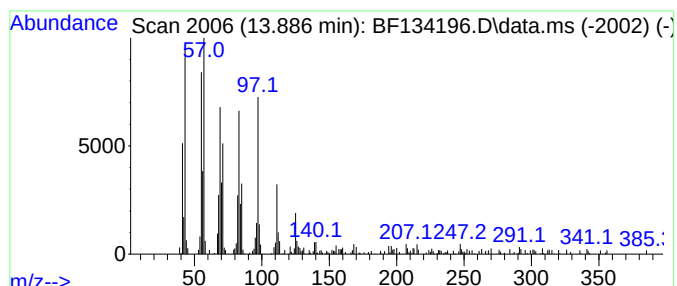
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclodocosane, ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	5.53 ng	186599	Chrysene-d12	14.033

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	99
2		1-Nonadecene	266	C19H38	018435-45-5	98
3		Cyclotetracosane	336	C24H48	000297-03-0	97
4		1-Octadecene	252	C18H36	000112-88-9	97
5		E-15-Heptadecenal	252	C17H32O	1000130-97-9	96



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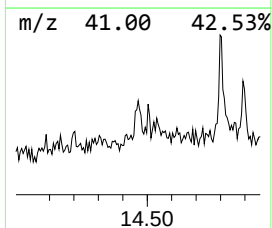
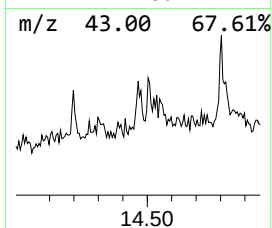
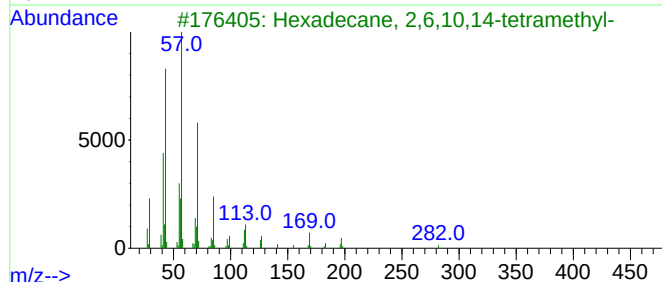
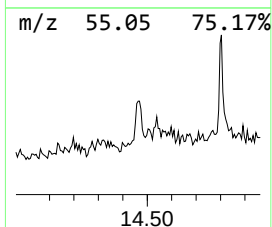
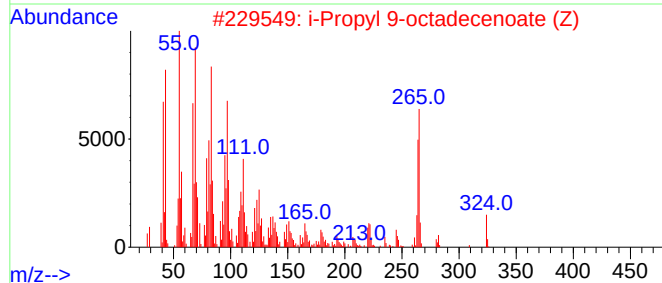
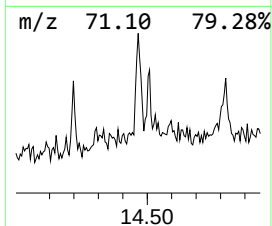
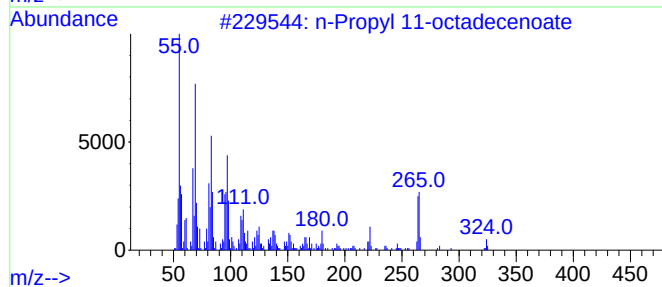
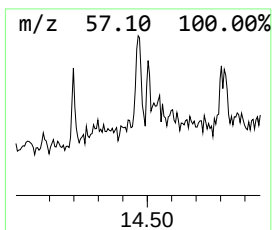
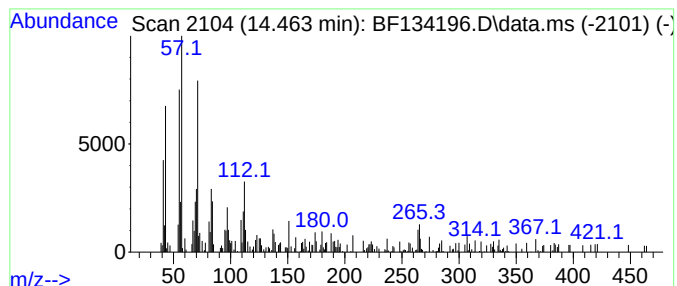
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Propyl 11-octadecenoate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.463	2.44 ng	82418	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Propyl 11-octadecenoate	324	C21H40O2	1000336-71-7	56
2			i-Propyl 9-octadecenoate (Z)	324	C21H40O2	000112-11-8	53
3			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	46
4			Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	43
5			Cycloundecanol, 1-methyl-	184	C12H24O	076154-15-9	38



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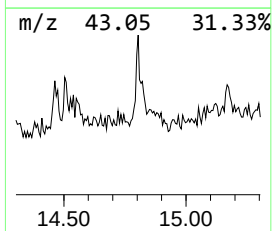
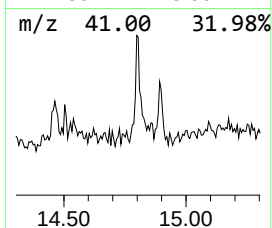
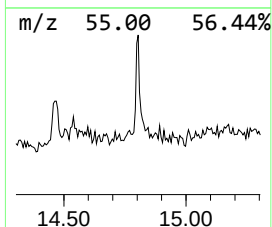
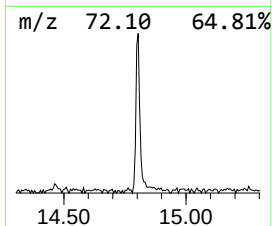
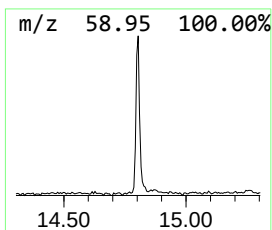
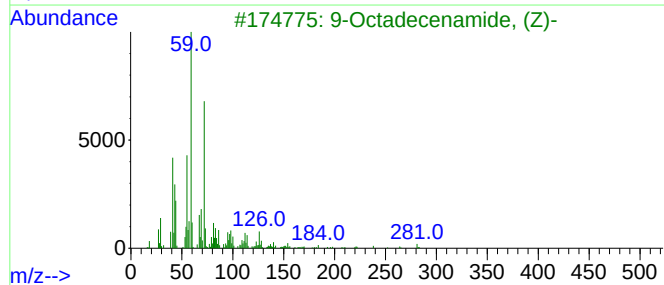
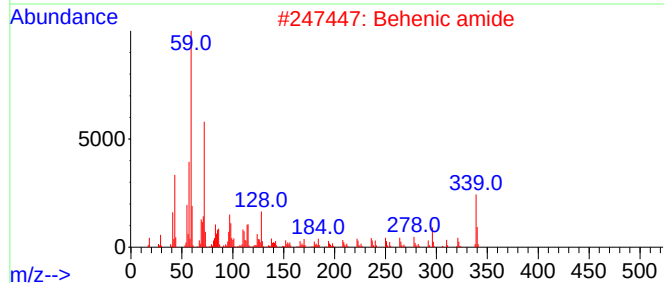
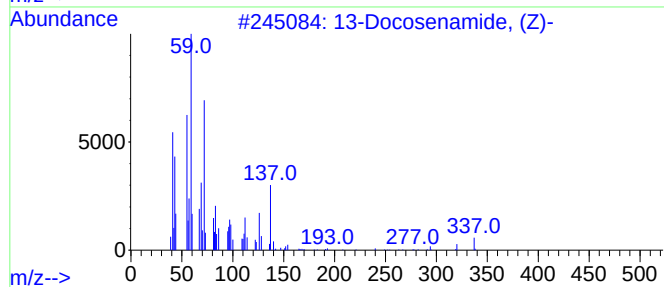
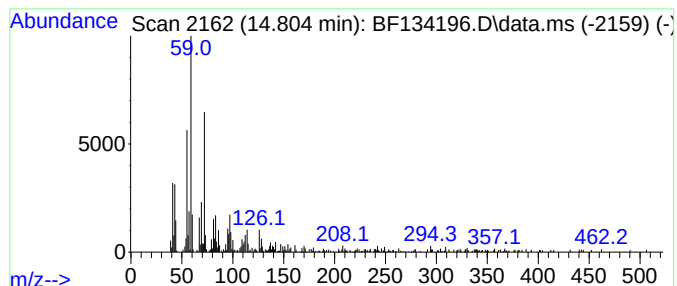
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	7.20 ng	191834	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2			Behenic amide	339	C22H45NO	003061-75-4	83
3			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	80
4			Dodecanamide	199	C12H25NO	001120-16-7	59
5			cis-11-Eicosenamide	309	C20H39NO	010436-08-5	55



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Sample : 03514-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CP-4

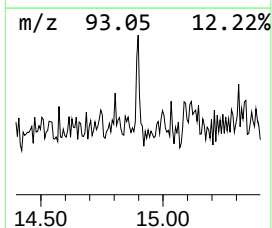
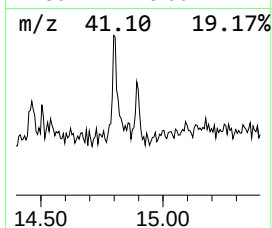
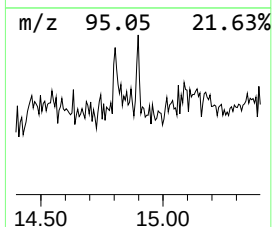
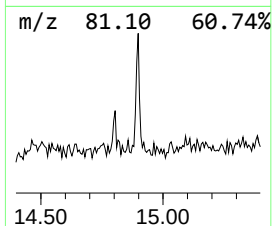
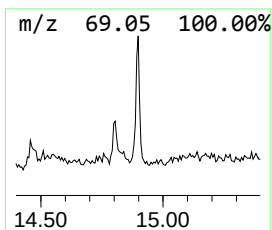
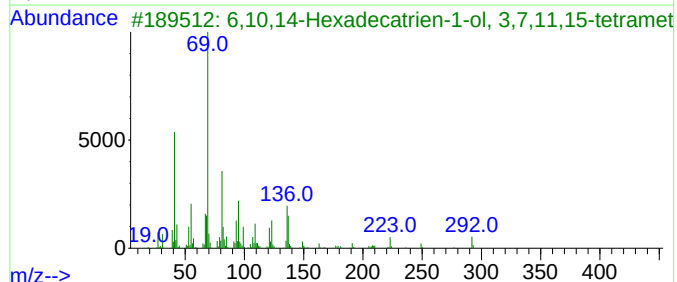
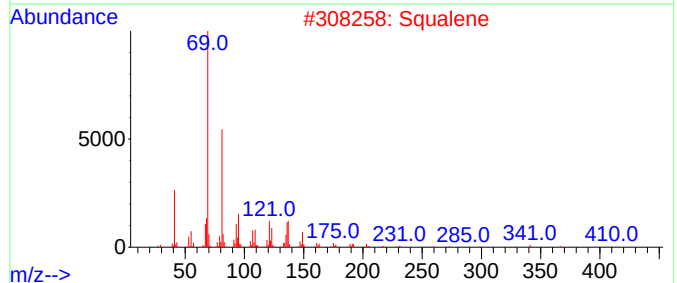
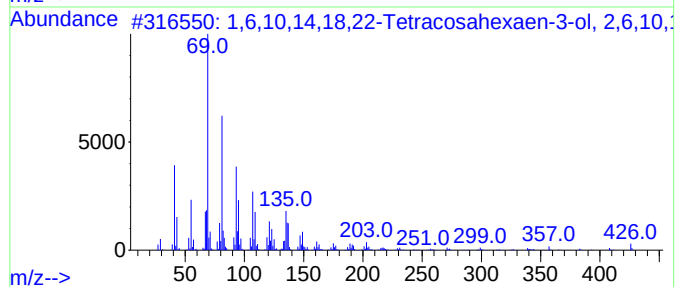
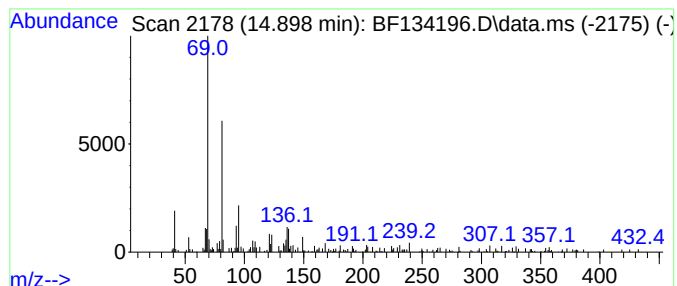
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,6,10,14,18,22-Tetracosahexa... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	2.50 ng	66623	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,10,14,18,22-Tetracosahexaen-...	426	C30H500	054159-46-5	72		
2	Squalene	410	C30H50	000111-02-4	72		
3	6,10,14-Hexadecatrien-1-ol, 3,7,...	292	C20H360	036237-66-8	72		
4	Supraene	410	C30H50	007683-64-9	64		
5	1,5-Heptadiene, 2,3,6-trimethyl-	138	C10H18	033501-88-1	59		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071023\
Data File : BF134196.D
Acq On : 10 Jul 2023 20:37
Operator : CG\JU
Sample : 03514-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.128	50.3	ng	1532060	1	6.845	608955	20.0
2-Pentanone, 4-...	5.081	3.7	ng	112203	1	6.845	608955	20.0
Benzophenone	10.598	3.5	ng	123110	3	9.881	694047	20.0
Cyclodocosane, ...	13.886	5.5	ng	186599	5	14.033	675241	20.0
n-Propyl 11-oct...	14.463	2.4	ng	82418	5	14.033	675241	20.0
13-Docosenamide...	14.804	7.2	ng	191834	6	15.539	533021	20.0
1,6,10,14,18,22...	14.898	2.5	ng	66623	6	15.539	533021	20.0