

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062923\
 Data File : BF134038.D
 Acq On : 29 Jun 2023 15:50
 Operator : CG\JU
 Sample : 03336-07
 Misc :
 ALS Vial : 12 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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134038.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	7	14	28	rVB	660172	997912	26.34%	4.256%
2	5.099	508	512	521	rVB	126062	186172	4.91%	0.794%
3	5.487	573	578	581	rBV	3167556	3249609	85.78%	13.860%
4	6.487	742	748	751	rBV	3114487	3237331	85.45%	13.807%
5	6.845	805	809	815	rBV	902952	721844	19.05%	3.079%
6	7.410	900	905	908	rBV	2395022	2186382	57.71%	9.325%
7	8.122	1023	1026	1030	rBV	1119442	962034	25.39%	4.103%
8	9.204	1206	1210	1213	rBV	4591936	3788367	100.00%	16.158%
9	9.881	1322	1325	1334	rBV	1139989	930178	24.55%	3.967%
10	10.598	1444	1447	1453	rBV	305991	243883	6.44%	1.040%
11	10.675	1456	1460	1473	rBV	1869367	1722343	45.46%	7.346%
12	11.375	1575	1579	1586	rBV	858742	752093	19.85%	3.208%
13	11.904	1666	1669	1678	rBV2	36822	63391	1.67%	0.270%
14	12.975	1847	1851	1854	rBV	3374750	3004082	79.30%	12.813%
15	13.892	2003	2007	2017	rBV2	116608	248919	6.57%	1.062%
16	14.033	2028	2031	2039	rVB	538294	540294	14.26%	2.304%
17	14.804	2159	2162	2169	rBV2	74998	102784	2.71%	0.438%
18	15.174	2223	2225	2230	rVB2	56227	70209	1.85%	0.299%
19	15.539	2283	2287	2297	rVB	311740	438551	11.58%	1.870%

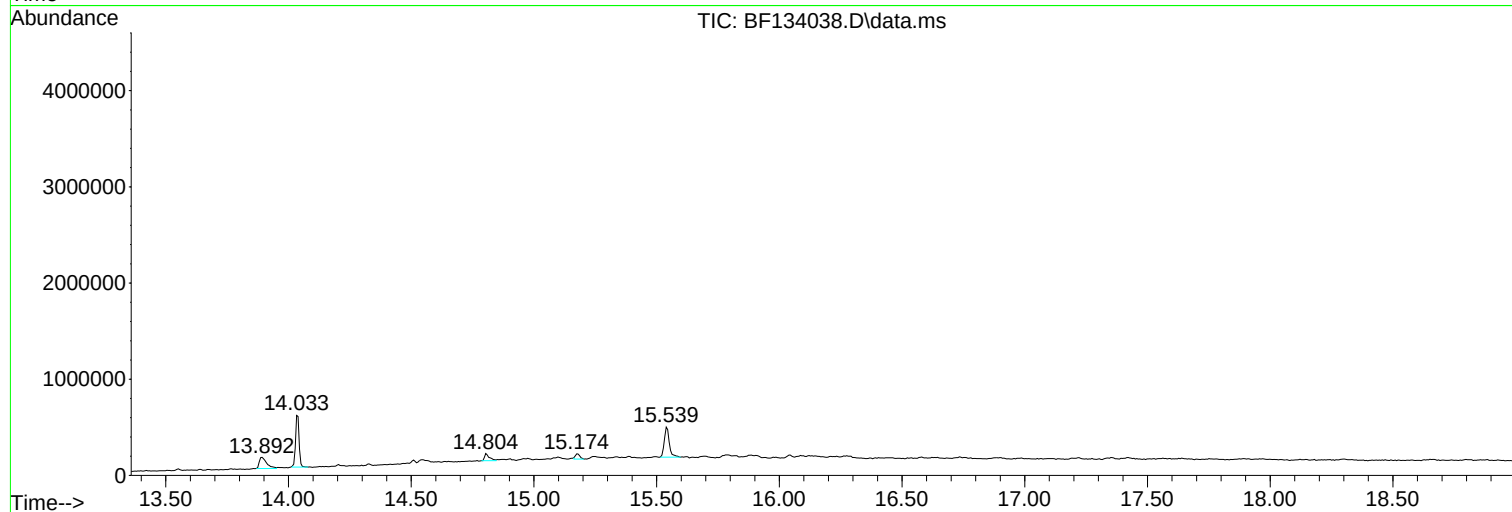
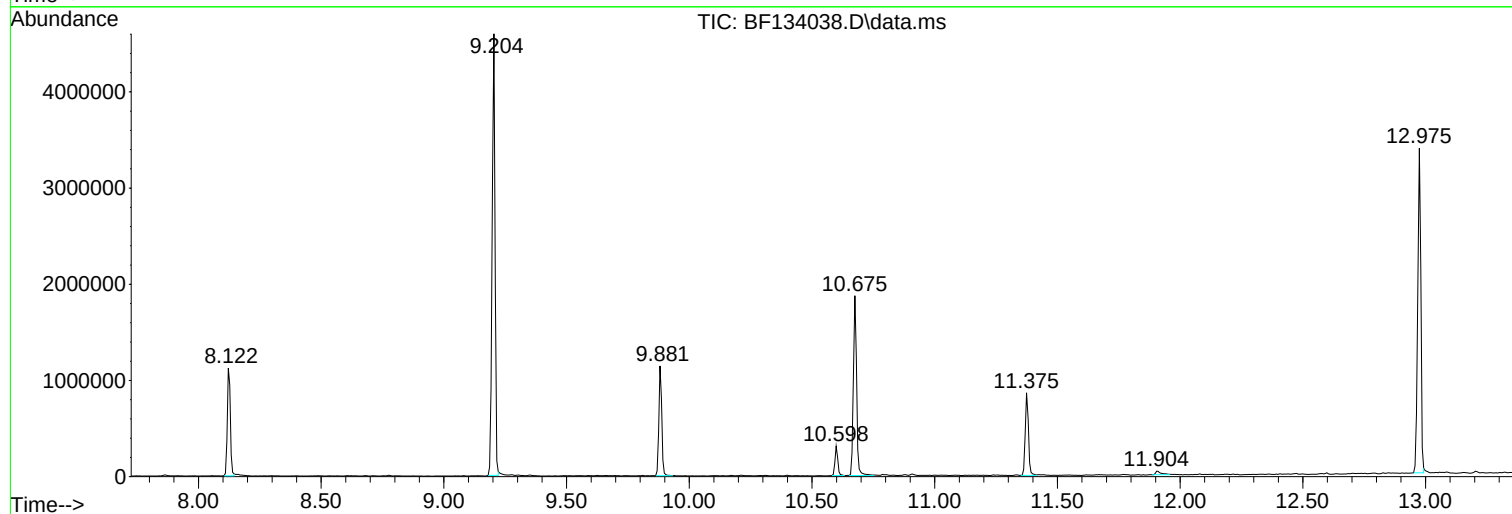
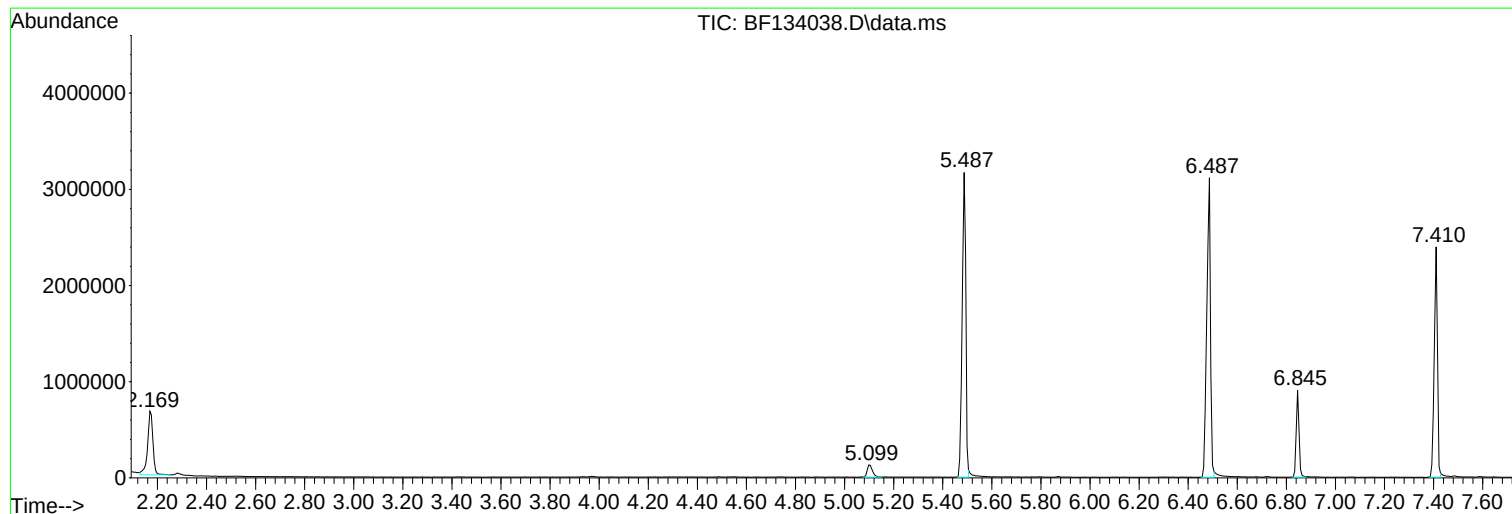
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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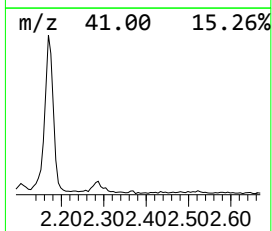
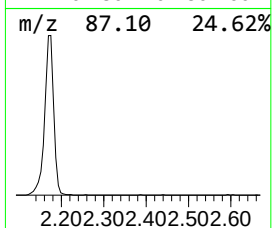
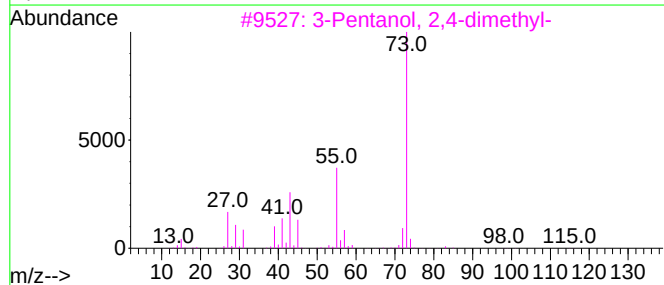
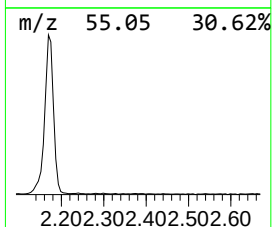
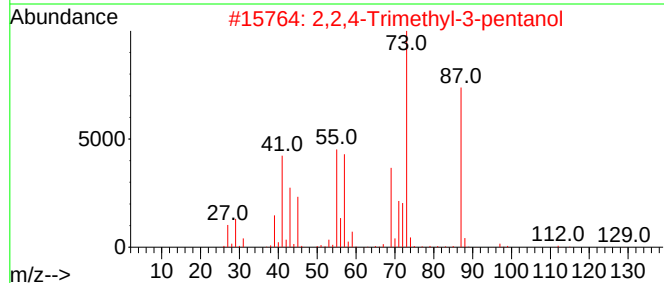
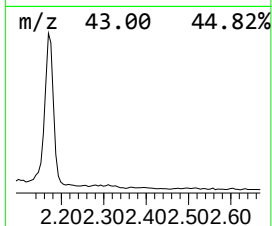
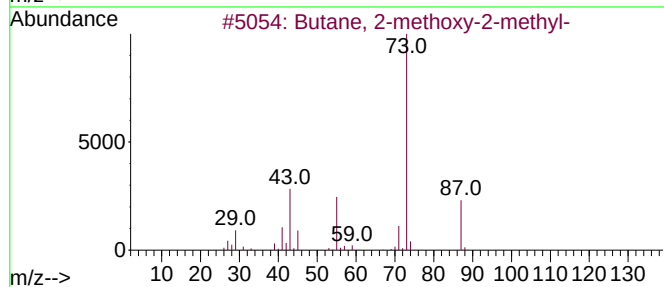
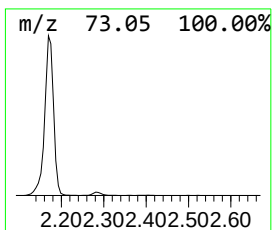
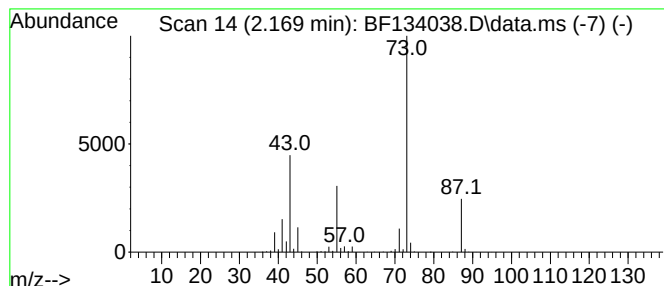
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	27.65 ng	997912	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			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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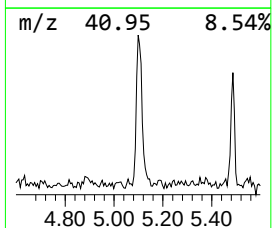
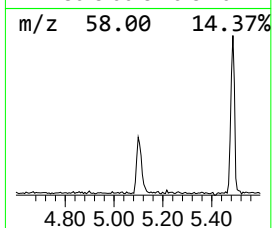
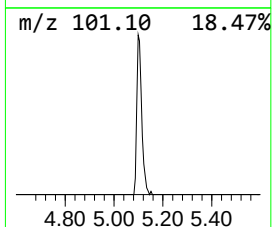
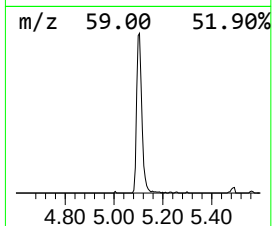
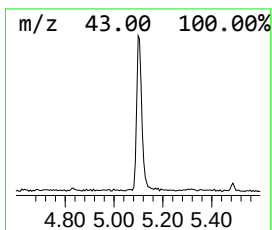
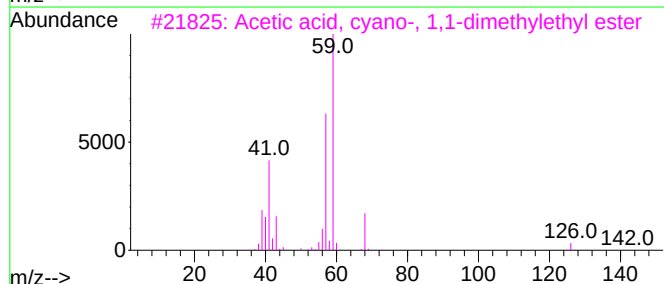
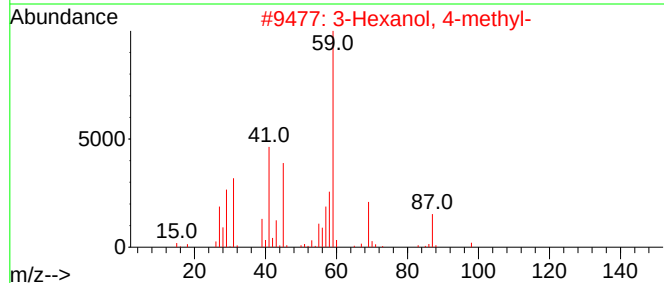
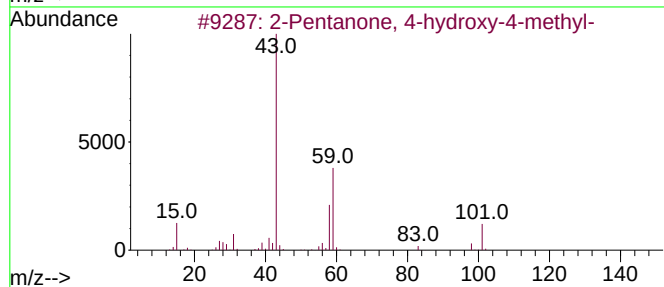
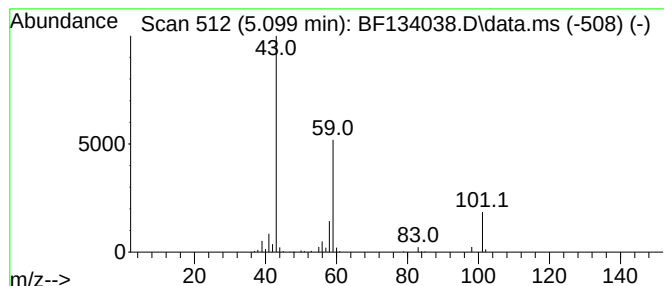
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.099	5.16 ng	186172	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	64	
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16	
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12	



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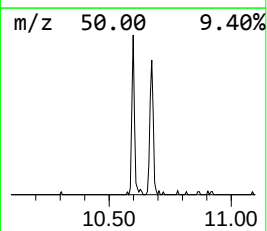
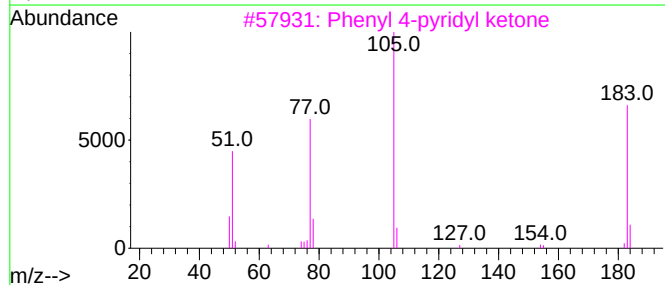
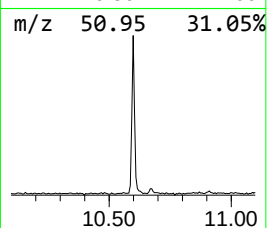
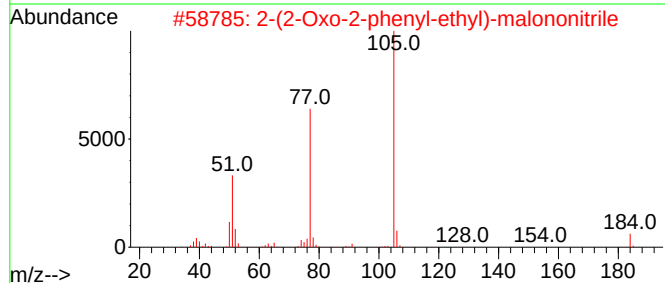
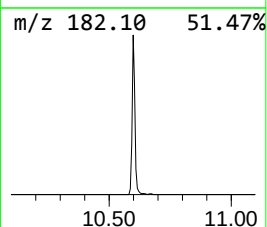
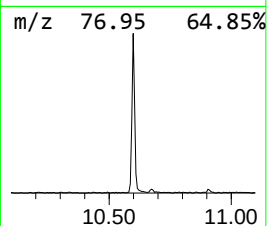
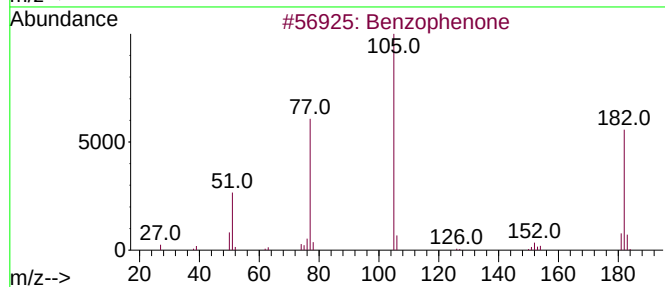
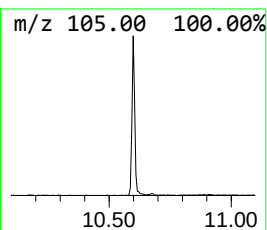
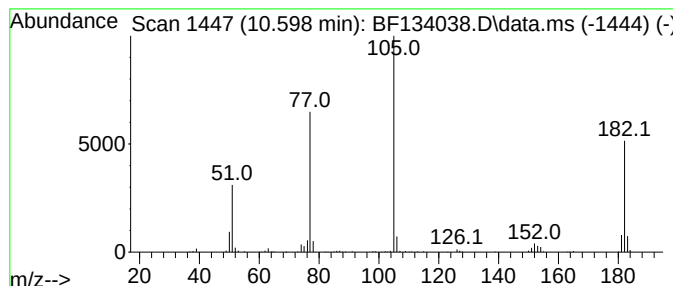
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.598	5.24 ng	243883	Acenaphthene-d10	9.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	58
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	52
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	50
5			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50



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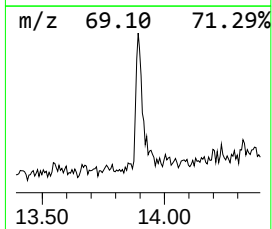
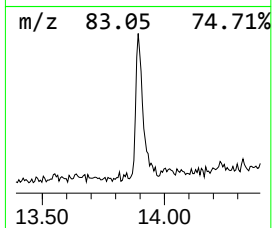
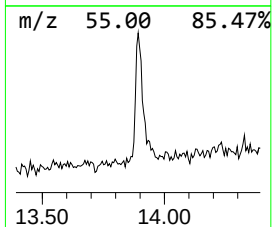
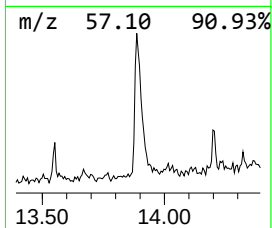
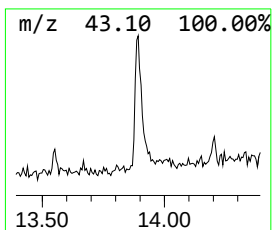
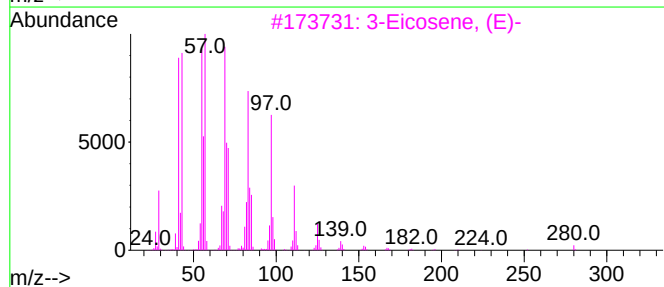
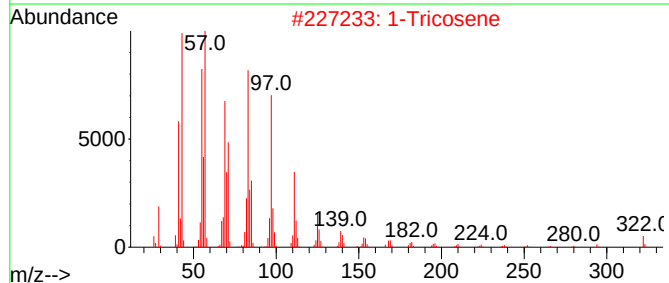
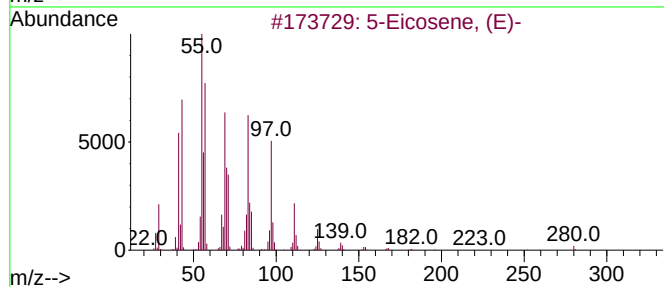
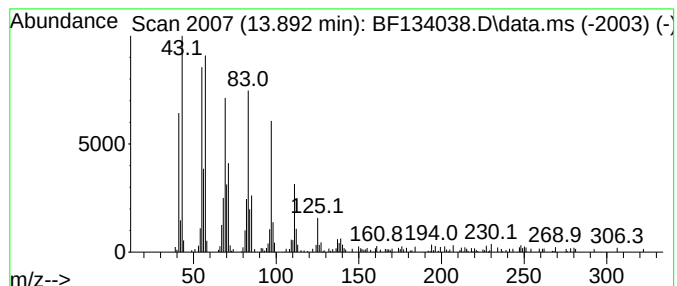
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Peak Number 4 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	9.21 ng	248919	Chrysene-d12	14.039

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	99
2	1-Tricosene		322	C23H46	018835-32-0	97
3	3-Eicosene, (E)-		280	C20H40	074685-33-9	96
4	1-Eicosene		280	C20H40	003452-07-1	95
5	Cyclohexadecane, 1,2-diethyl-		280	C20H40	1000155-85-3	94



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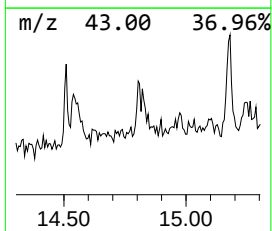
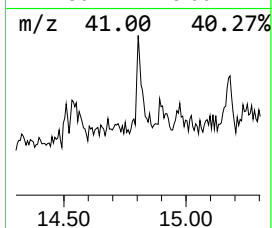
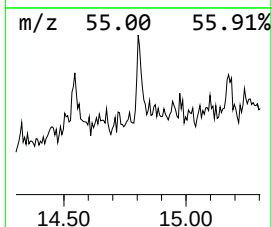
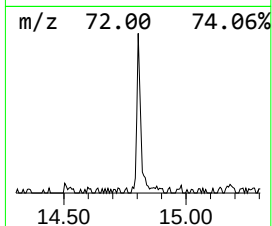
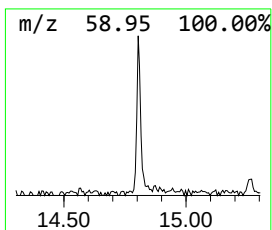
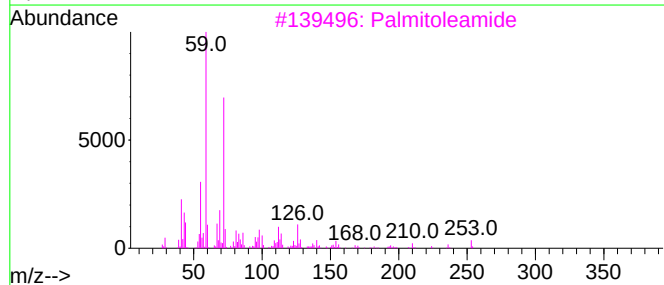
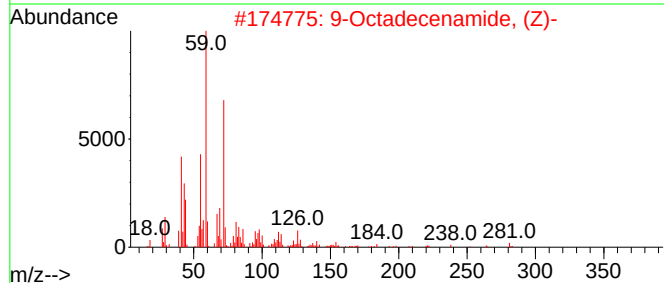
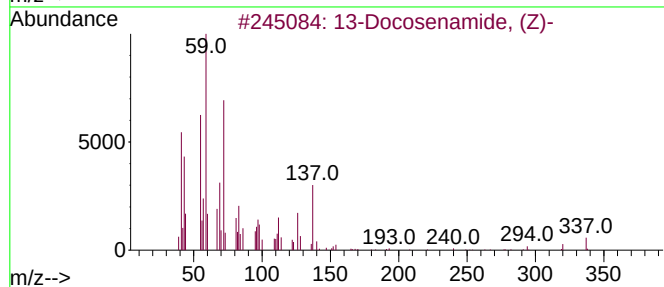
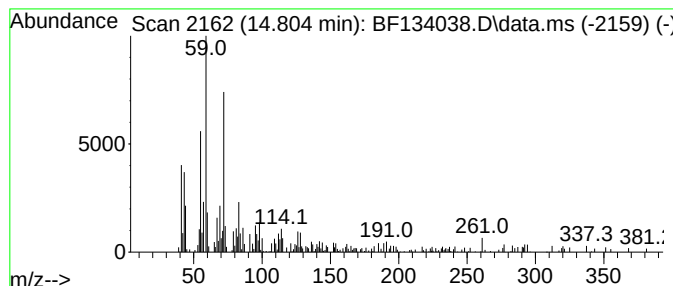
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Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	4.69 ng	102784	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	83
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	80
3			Palmitoleamide	253	C16H31NO	106010-22-4	80
4			Tetradecanamide	227	C14H29NO	000638-58-4	52
5			Octadecanamide	283	C18H37NO	000124-26-5	45



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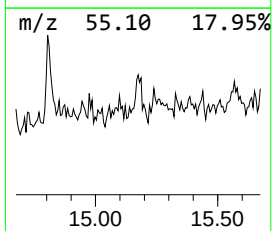
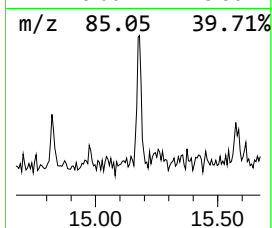
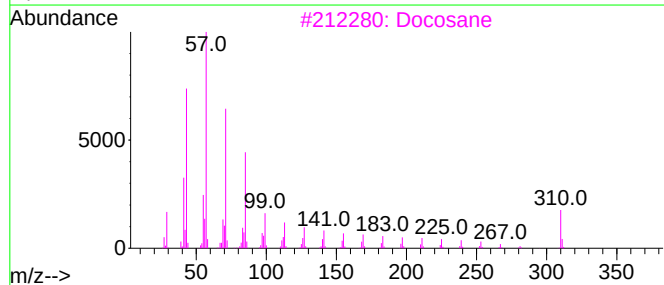
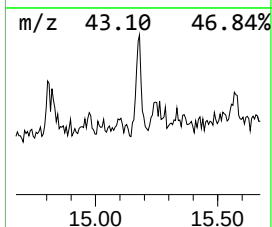
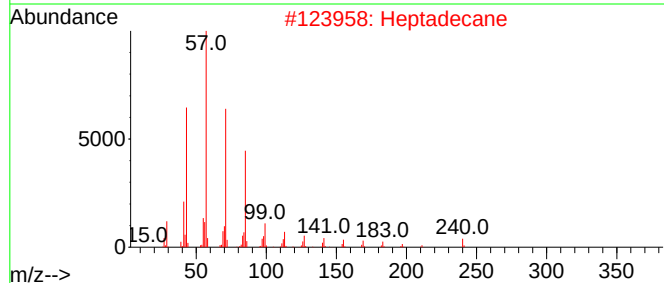
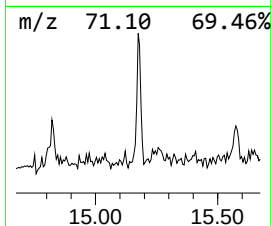
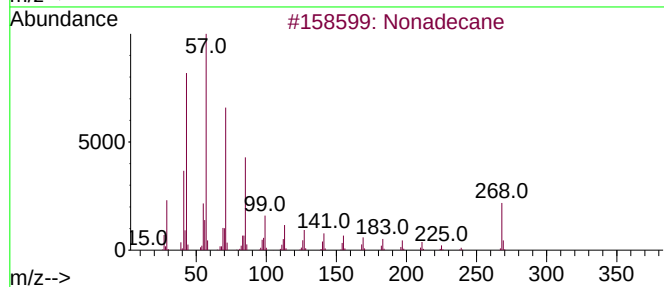
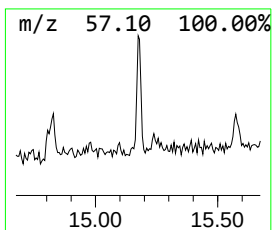
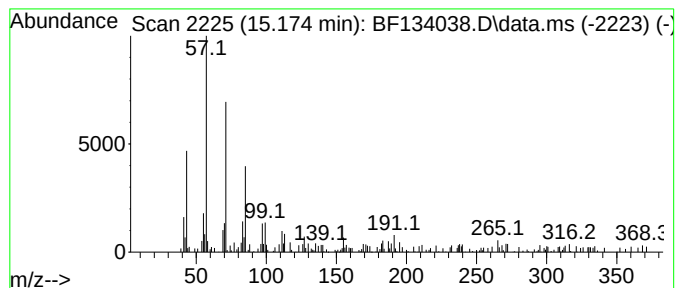
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	3.20 ng	70209	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	93
2			Heptadecane	240	C17H36	000629-78-7	92
3			Docosane	310	C22H46	000629-97-0	91
4			9-Methylheneicosane	310	C22H46	070475-51-3	90
5			Tricosane	324	C23H48	000638-67-5	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062923\
Data File : BF134038.D
Acq On : 29 Jun 2023 15:50
Operator : CG\JU
Sample : 03336-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-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\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.169	27.6	ng	997912	1	6.845	721844	20.0
2-Pentanone, 4-...	5.099	5.2	ng	186172	1	6.845	721844	20.0
Benzophenone	10.598	5.2	ng	243883	3	9.881	930178	20.0
5-Eicosene, (E)-	13.892	9.2	ng	248919	5	14.039	540294	20.0
13-Docosenamide...	14.804	4.7	ng	102784	6	15.539	438551	20.0
Nonadecane	15.174	3.2	ng	70209	6	15.539	438551	20.0