

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070523\
 Data File : BF134077.D
 Acq On : 05 Jul 2023 20:59
 Operator : CG\JU
 Sample : 03483-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RO-CHRT-24801

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: BF134077.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	7	15	27	rVB	1060712	1416986	37.65%	4.629%
2	2.287	30	34	41	rVB2	25406	41031	1.09%	0.134%
3	5.104	503	513	521	rBV	120245	183478	4.87%	0.599%
4	5.487	573	578	582	rBV	2870852	3105945	82.52%	10.146%
5	6.486	743	748	751	rBV	2854300	3156446	83.86%	10.310%
6	6.845	805	809	818	rBV	1010814	814099	21.63%	2.659%
7	7.410	900	905	908	rBV	2078856	2086215	55.43%	6.815%
8	8.128	1023	1027	1030	rBV	1218711	1037129	27.55%	3.388%
9	9.204	1206	1210	1213	rBV	4237692	3763967	100.00%	12.295%
10	9.886	1322	1326	1329	rBV	1277529	1088513	28.92%	3.556%
11	10.598	1444	1447	1455	rBV	488757	445437	11.83%	1.455%
12	10.680	1456	1461	1473	rVV	1732328	1690599	44.92%	5.522%
13	10.910	1497	1500	1504	rVB	81301	66039	1.75%	0.216%
14	11.380	1576	1580	1582	rBV	1216791	1036539	27.54%	3.386%
15	11.404	1582	1584	1587	rVB	260275	211847	5.63%	0.692%
16	11.486	1595	1598	1601	rVB	46463	41490	1.10%	0.136%
17	11.616	1613	1620	1626	rBV	22482	45845	1.22%	0.150%
18	11.910	1660	1670	1681	rBV	611140	802141	21.31%	2.620%
19	11.992	1681	1684	1687	rBV	65553	63811	1.70%	0.208%
20	12.598	1784	1787	1790	rBV	584379	550542	14.63%	1.798%
21	12.704	1799	1805	1817	rVV	684399	842375	22.38%	2.752%
22	12.833	1821	1827	1832	rVV	439902	553825	14.71%	1.809%
23	12.880	1832	1835	1839	rVB3	31380	45771	1.22%	0.150%
24	12.980	1847	1852	1855	rBV	3246258	3030211	80.51%	9.898%
25	13.163	1881	1883	1886	rVB	62246	49058	1.30%	0.160%
26	13.551	1947	1949	1958	rVB3	29621	41000	1.09%	0.134%
27	13.674	1967	1970	1974	rVB	41018	43051	1.14%	0.141%
28	13.898	2003	2008	2016	rBV5	177338	391154	10.39%	1.278%
29	14.039	2025	2032	2035	rBV2	886502	1031860	27.41%	3.371%
30	14.062	2035	2036	2044	rVB	205086	167539	4.45%	0.547%
31	14.509	2109	2112	2114	rBV2	61635	58496	1.55%	0.191%
32	14.545	2114	2118	2127	rVB5	138205	321644	8.55%	1.051%
33	14.974	2188	2191	2201	rBV	261834	298150	7.92%	0.974%
34	15.098	2208	2212	2216	rBV	158363	245476	6.52%	0.802%
35	15.180	2222	2226	2229	rBV	87577	105674	2.81%	0.345%
36	15.227	2230	2234	2248	rVB3	216627	562201	14.94%	1.836%

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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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.409	2263	2265	2270	rVB	75994	93064	2.47%	0.304%
38	15.480	2273	2277	2283	rBV	108266	161464	4.29%	0.527%
39	15.545	2283	2288	2292	rBV	445089	588465	15.63%	1.922%
40	15.786	2327	2329	2335	rVB4	72888	105213	2.80%	0.344%
41	16.039	2367	2372	2377	rVB	140568	230189	6.12%	0.752%

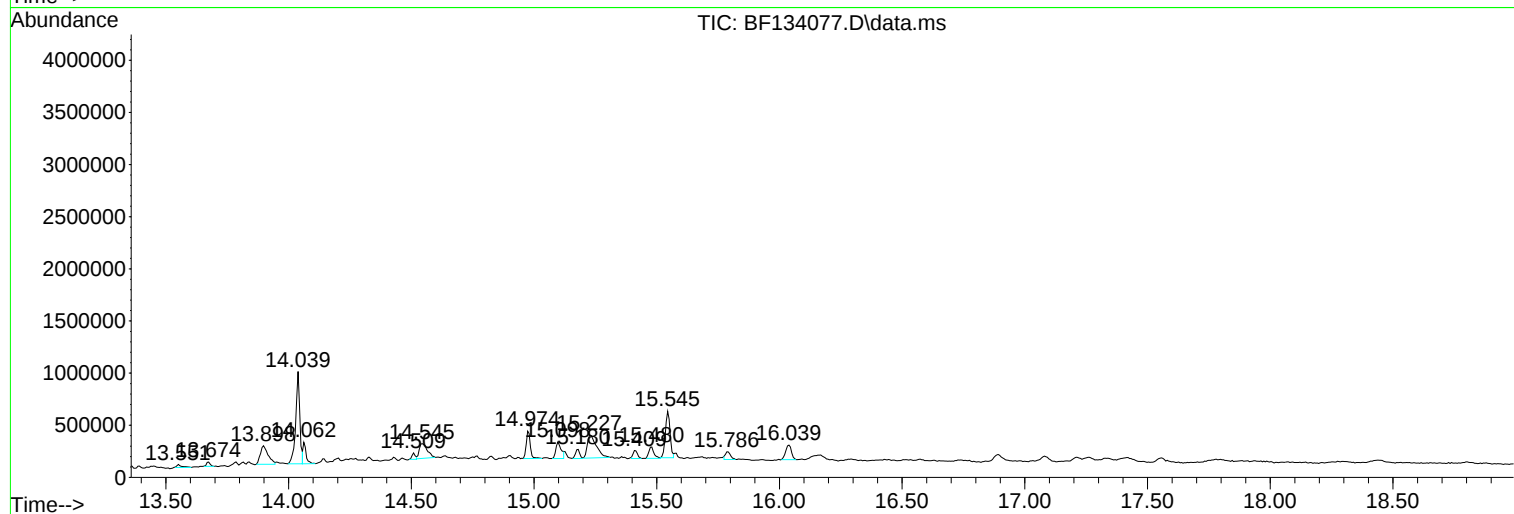
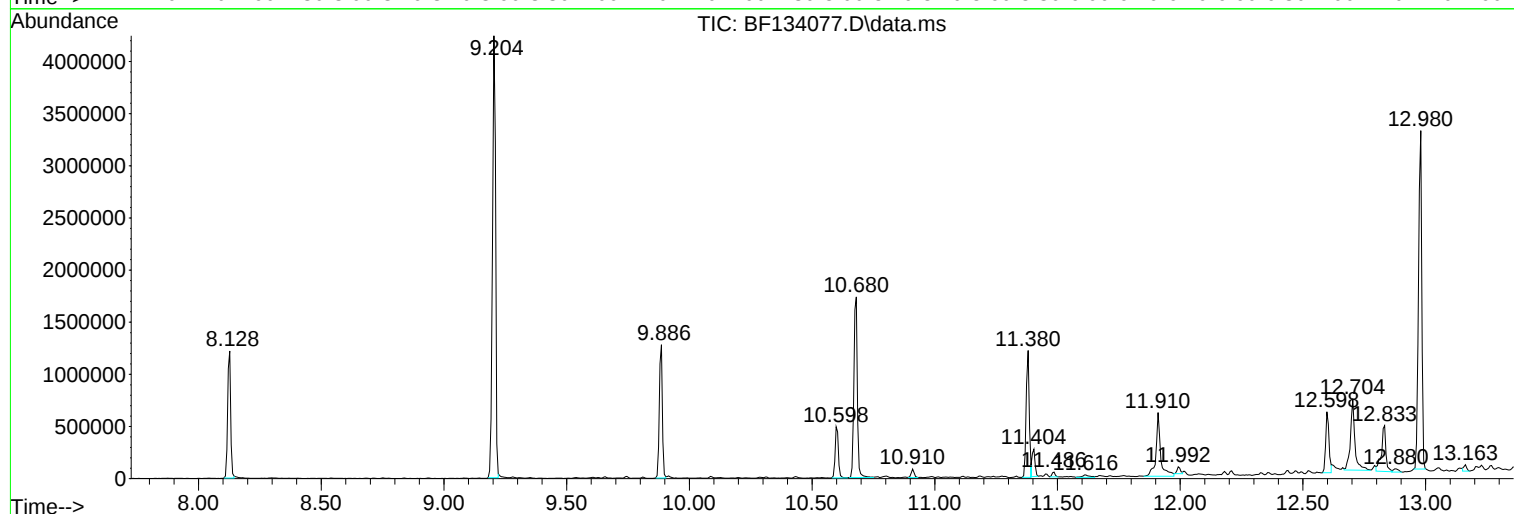
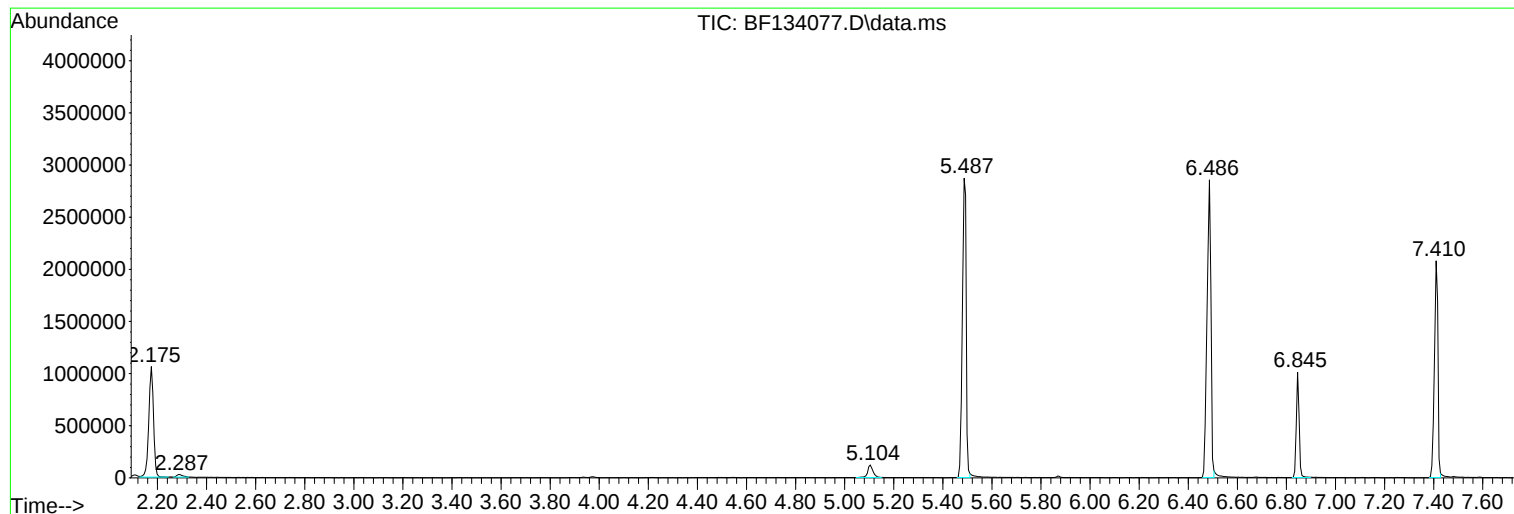
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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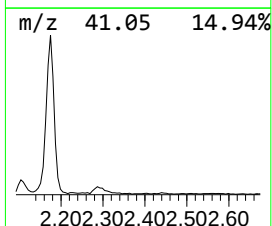
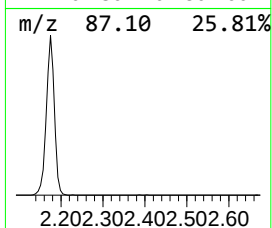
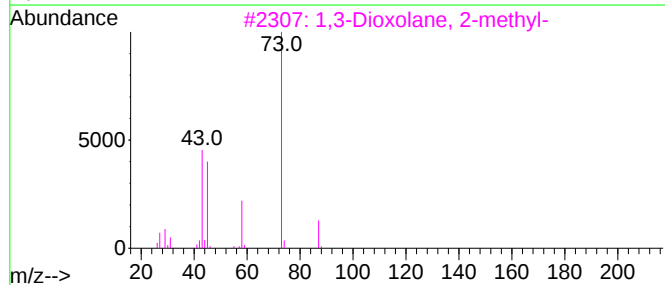
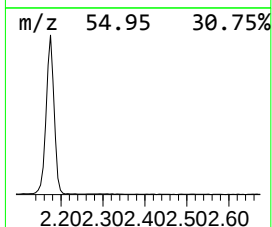
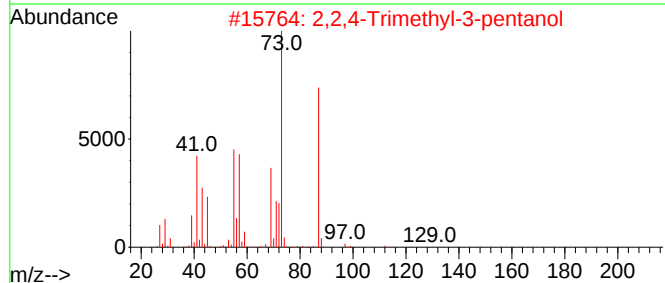
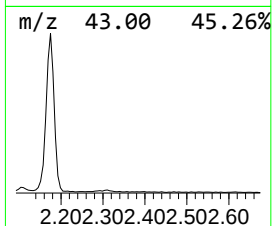
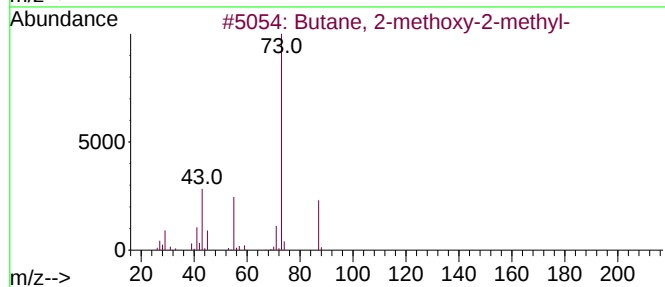
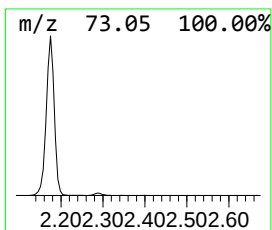
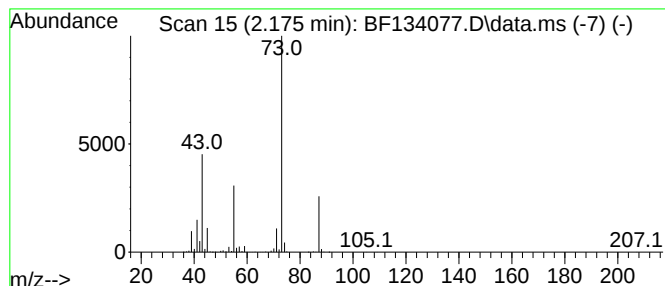
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	34.81 ng	1416990	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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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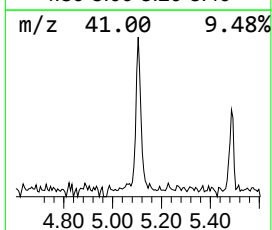
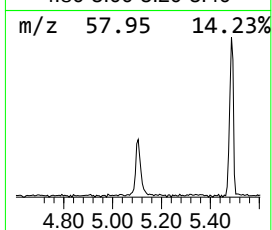
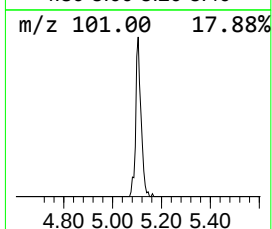
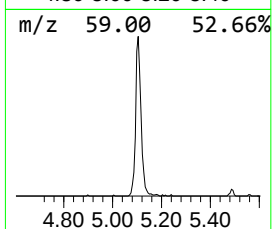
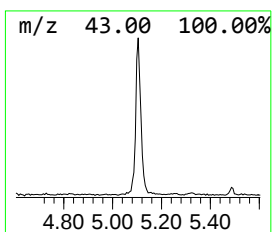
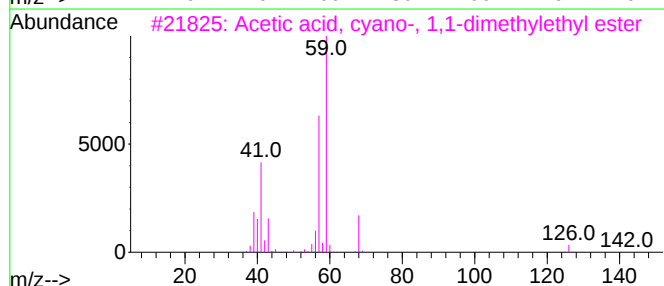
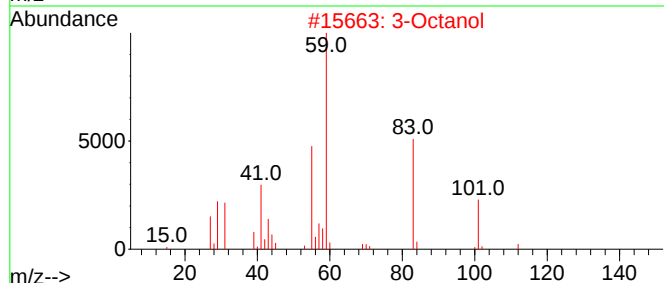
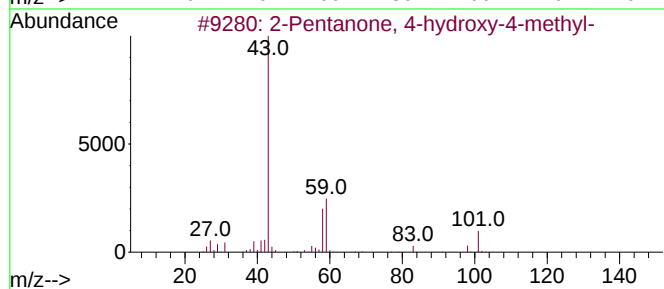
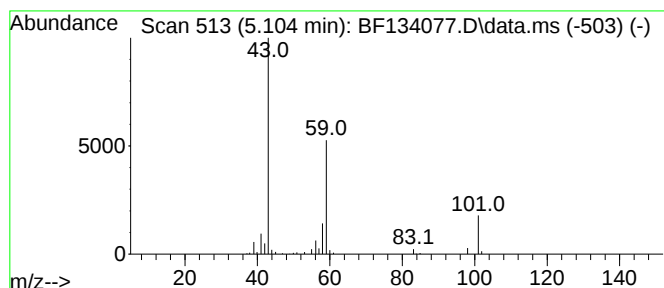
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	4.51 ng	183478	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-Octanol	130	C8H18O	000589-98-0	36	
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9	



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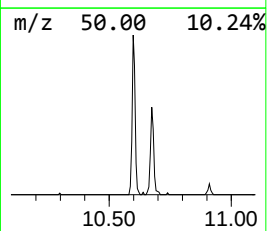
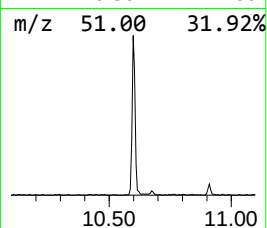
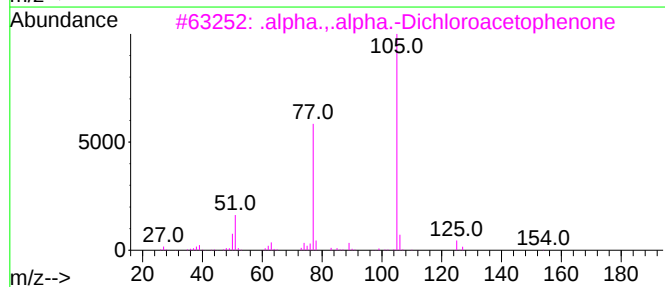
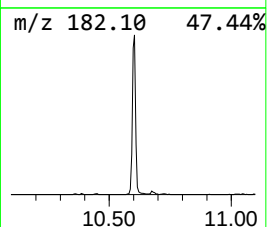
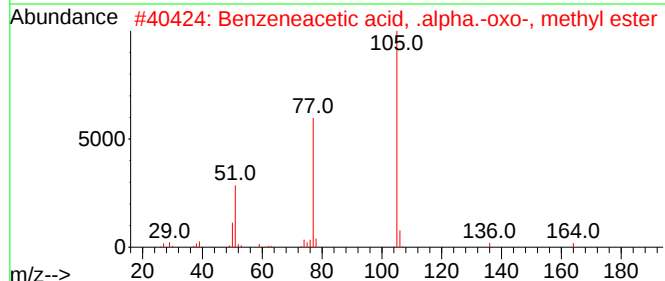
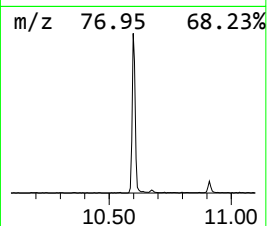
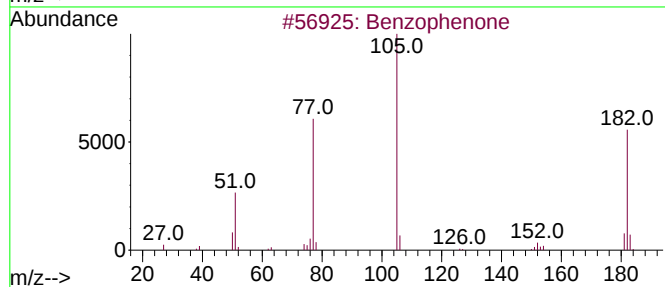
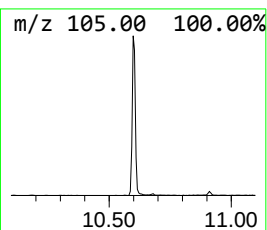
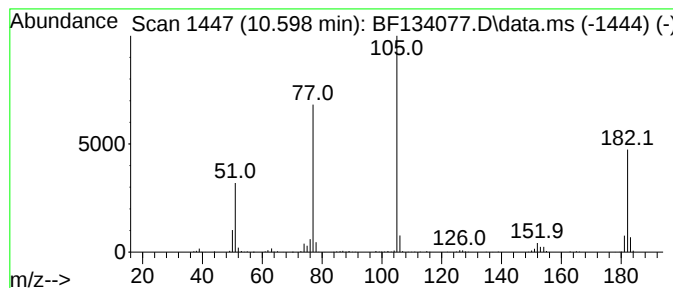
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.598	8.18 ng	445437	Acenaphthene-d10	9.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	50
3			.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	50
4			2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	50
5			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	50



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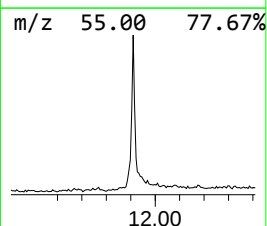
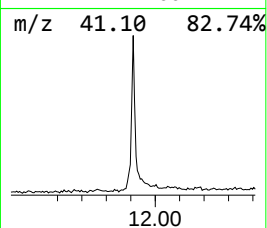
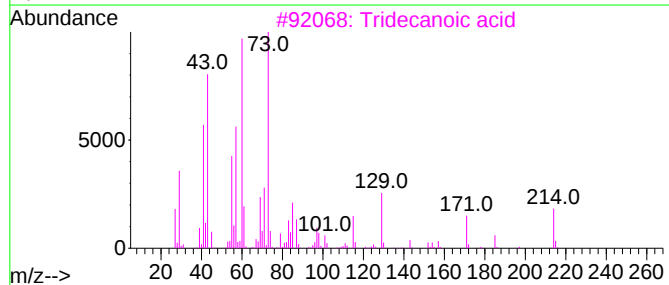
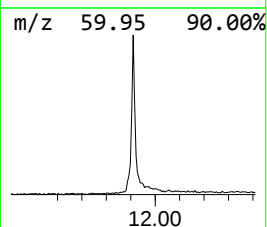
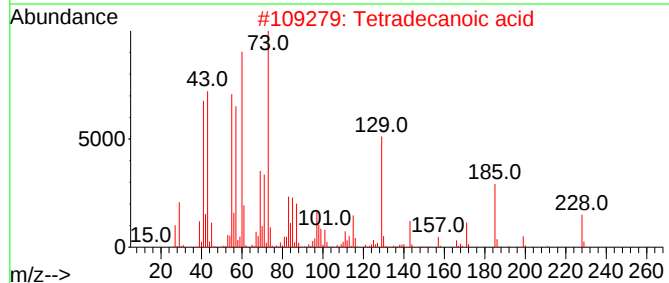
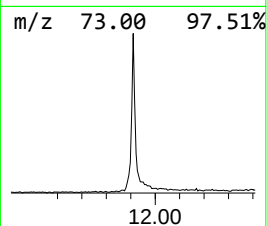
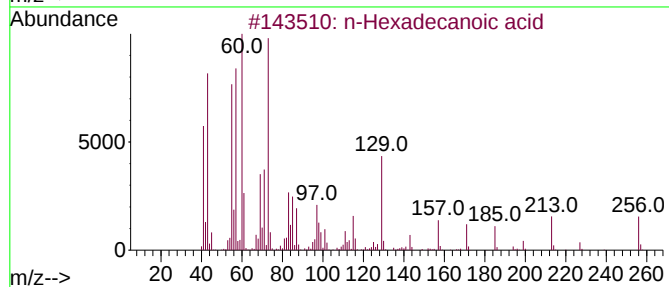
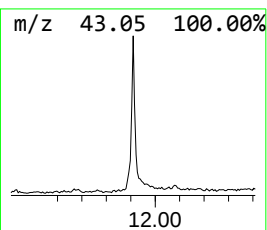
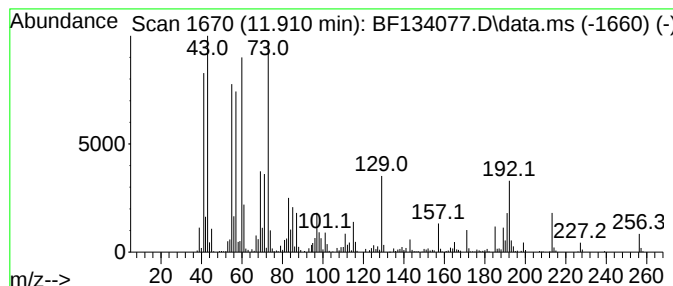
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	15.48 ng	802141	Phenanthrene-d10	11.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	92
3			Tridecanoic acid	214	C13H26O2	000638-53-9	76
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5			Undecanoic acid	186	C11H22O2	000112-37-8	58



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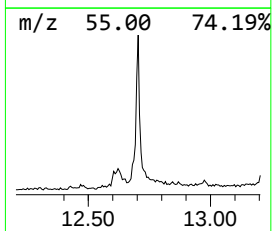
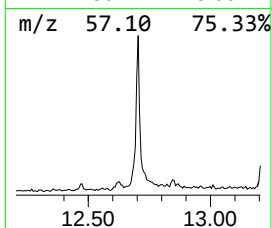
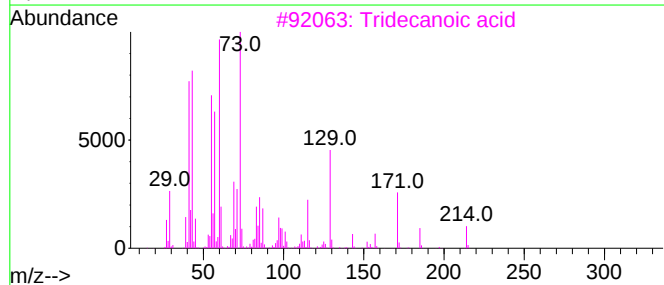
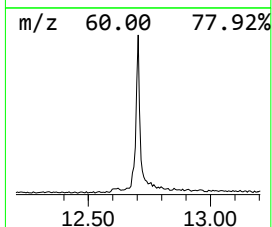
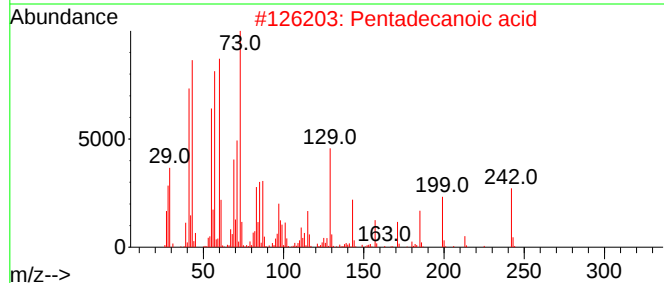
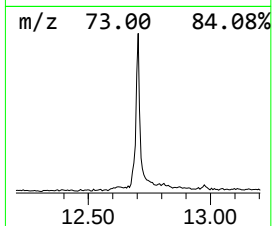
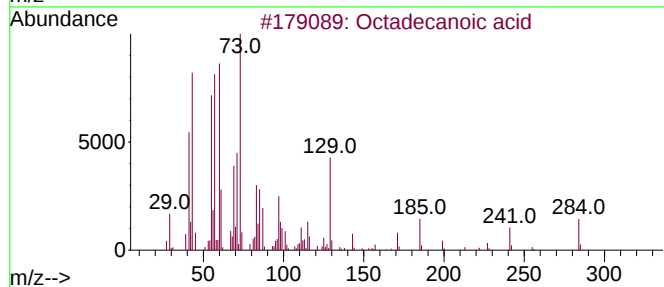
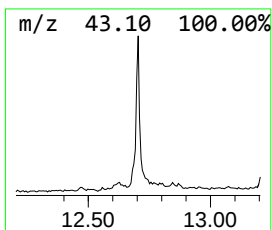
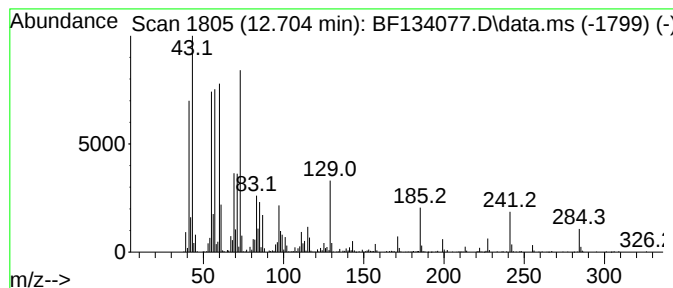
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	16.25 ng	842375	Phenanthrene-d10	11.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3			Tridecanoic acid	214	C13H26O2	000638-53-9	76
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070523\
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Acq On : 05 Jul 2023 20:59
Operator : CG\JU
Sample : 03483-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
RO-CHRT-24801

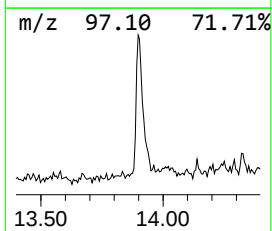
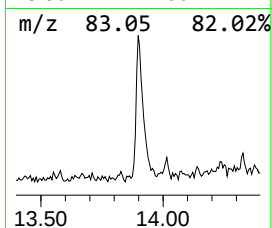
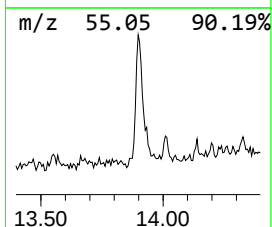
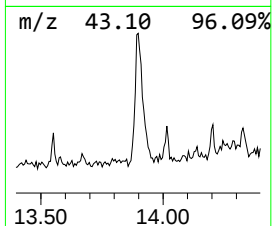
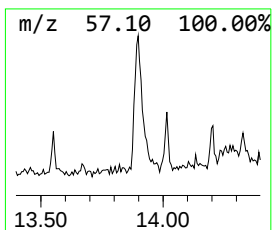
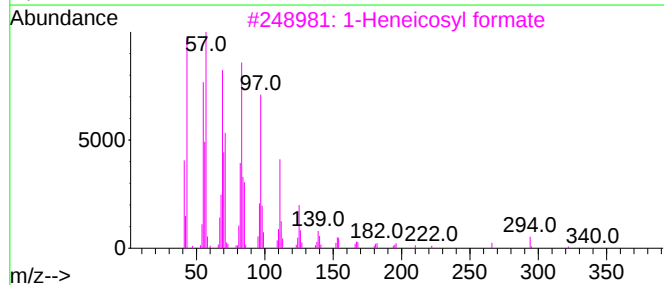
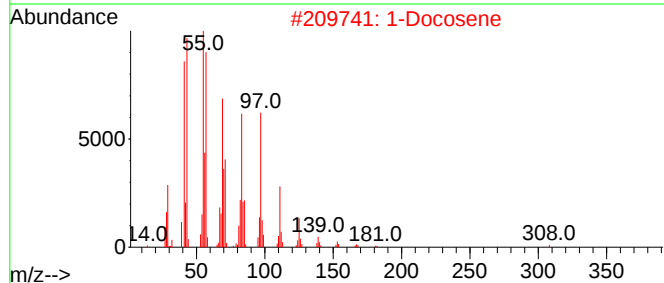
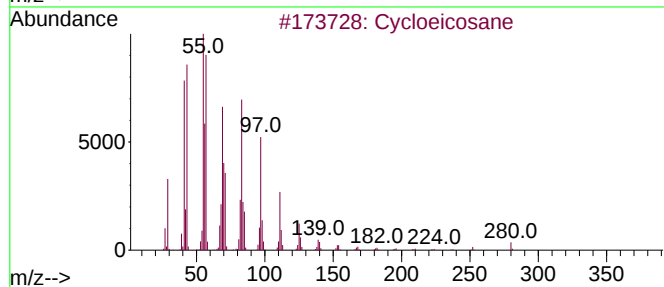
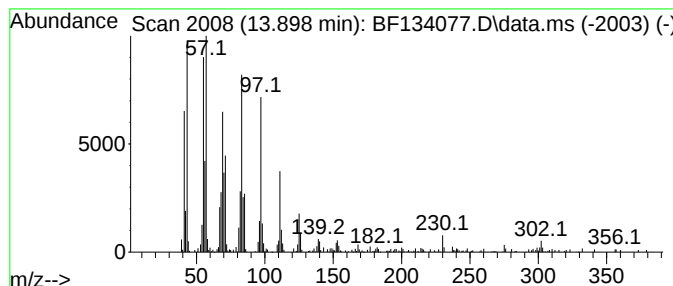
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cycloeicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	7.58 ng	391154	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloeicosane	280	C20H40	000296-56-0	98
2			1-Docosene	308	C22H44	001599-67-3	97
3			1-Heneicosyl formate	340	C22H44O2	077899-03-7	96
4			1-Tetracosene	336	C24H48	010192-32-2	95
5			Cyclotetracosane	336	C24H48	000297-03-0	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070523\
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ClientSampleId :
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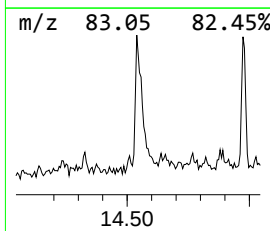
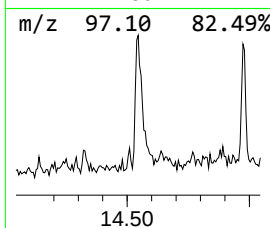
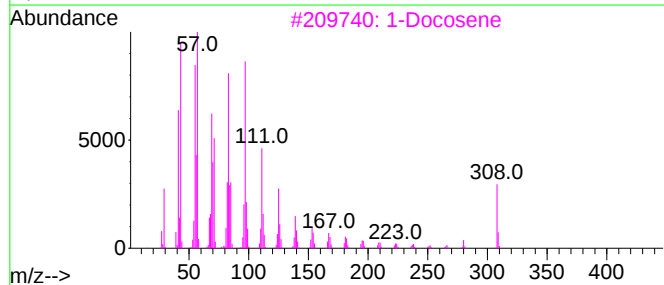
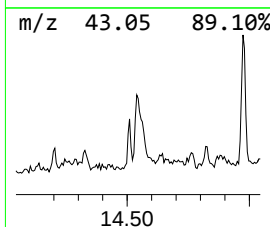
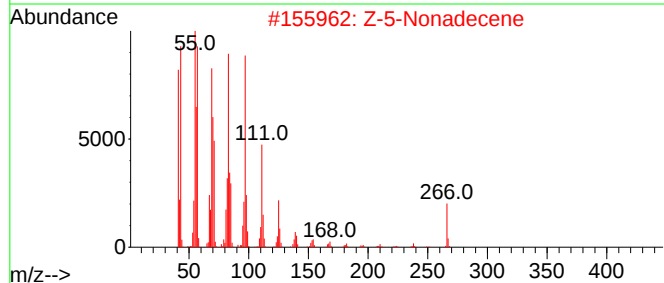
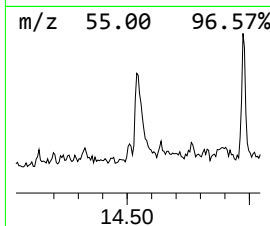
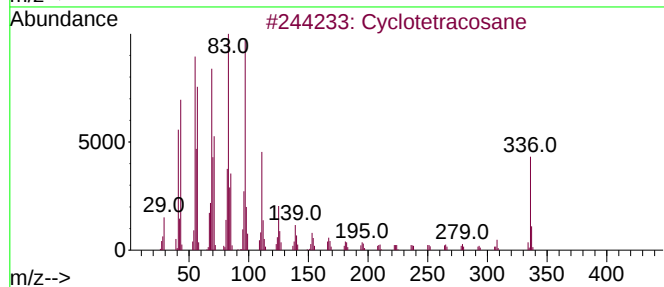
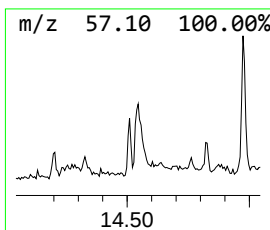
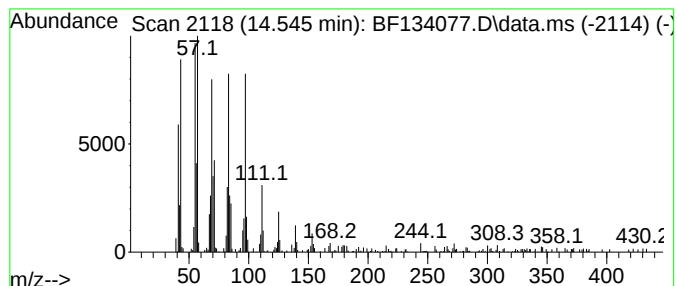
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclotetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.545	6.23 ng	321644	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	97
2			Z-5-Nonadecene	266	C19H38	1000131-11-8	96
3			1-Docosene	308	C22H44	001599-67-3	95
4			1-Nonadecene	266	C19H38	018435-45-5	95
5			1-Pentadecanethiol	244	C15H32S	025276-70-4	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070523\
Data File : BF134077.D
Acq On : 05 Jul 2023 20:59
Operator : CG\JU
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Misc :
ALS Vial : 6 Sample Multiplier: 1

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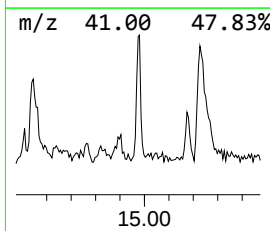
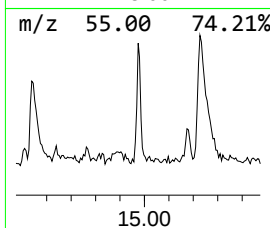
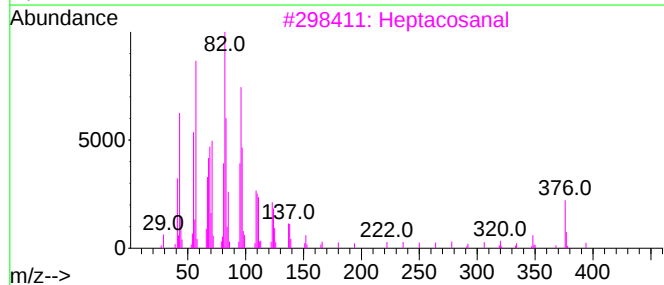
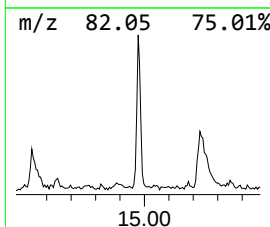
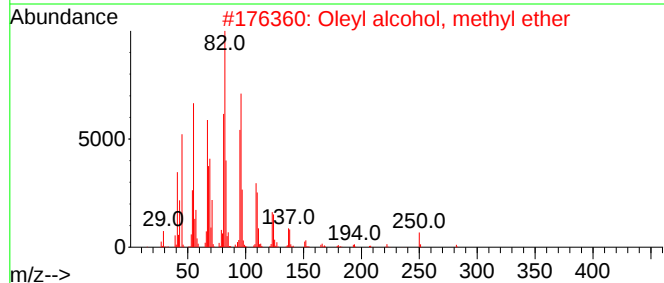
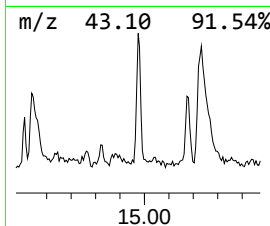
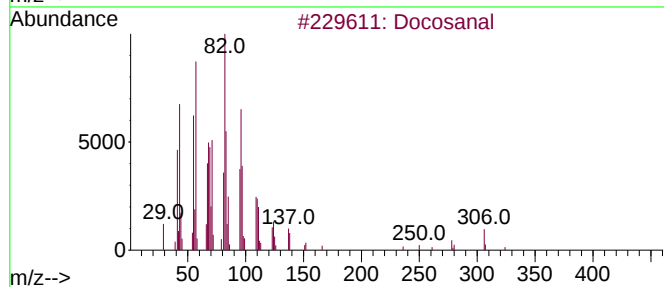
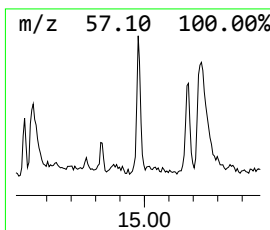
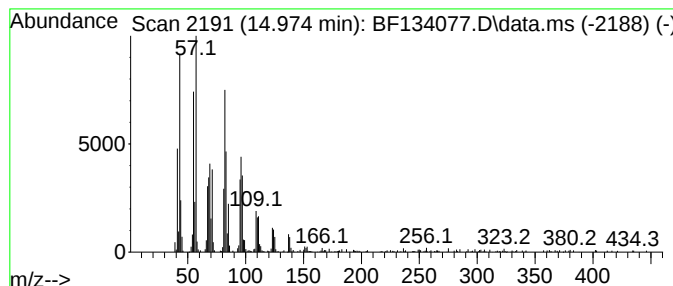
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Docosanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.974	10.13 ng	298150	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosanal	324	C22H44O	057402-36-5	94
2			Oleyl alcohol, methyl ether	282	C19H38O	1010352-68-0	93
3			Heptacosanal	394	C27H54O	072934-03-3	91
4			Octadecanal	268	C18H36O	000638-66-4	91
5			Heptadecanal	254	C17H34O	1000376-70-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070523\
Data File : BF134077.D
Acq On : 05 Jul 2023 20:59
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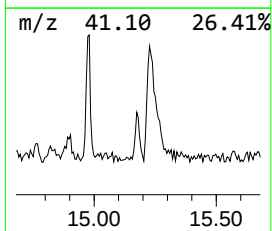
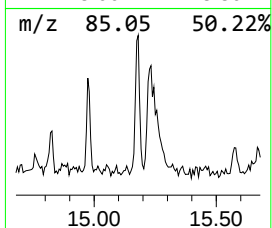
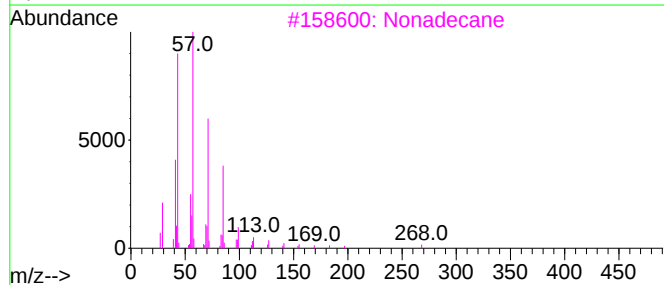
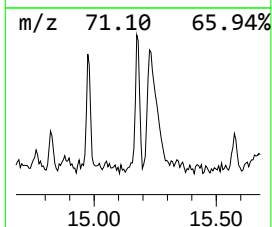
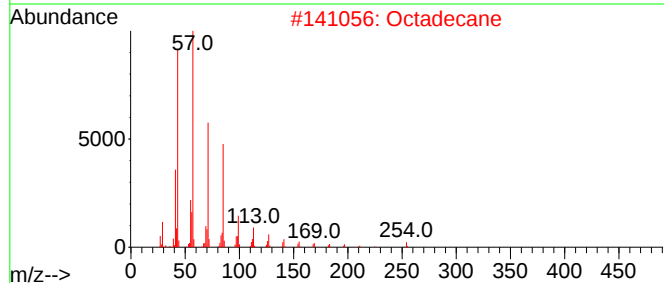
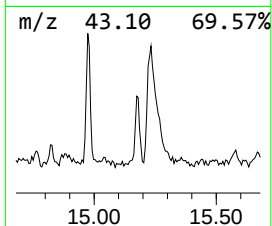
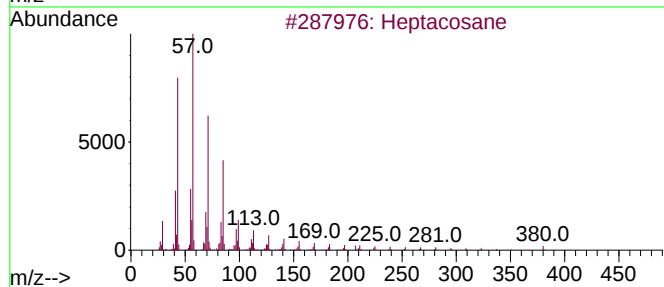
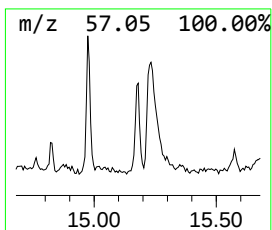
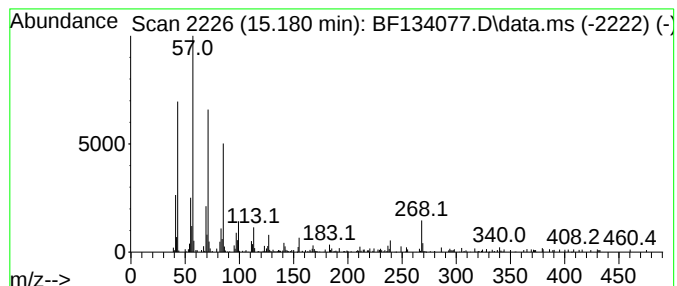
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.180	3.59 ng	105674	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	96
2			Octadecane	254	C18H38	000593-45-3	95
3			Nonadecane	268	C19H40	000629-92-5	93
4			Tetracosane	338	C24H50	000646-31-1	93
5			Nonacosane	408	C29H60	000630-03-5	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070523\
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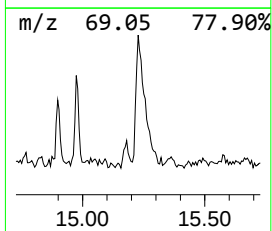
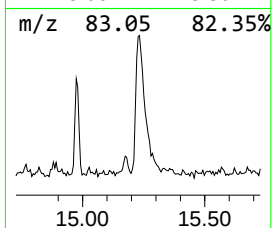
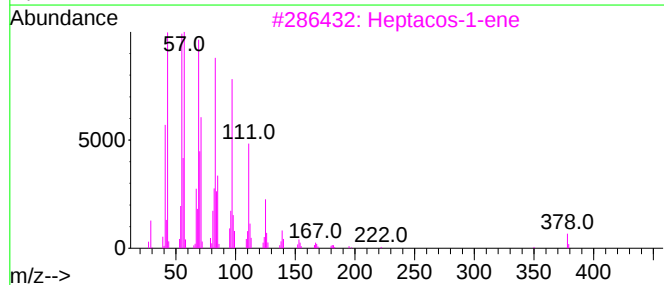
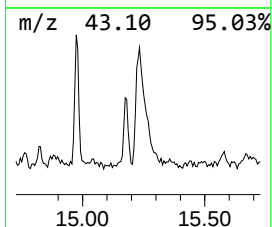
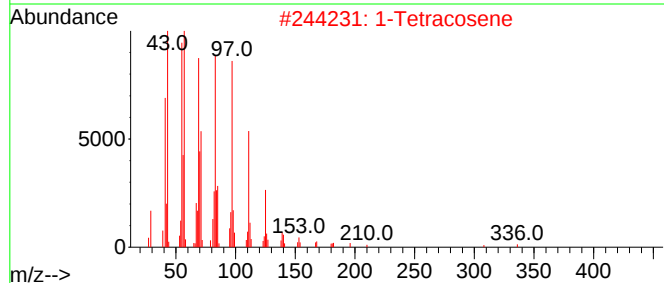
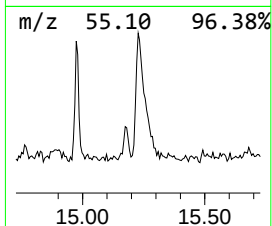
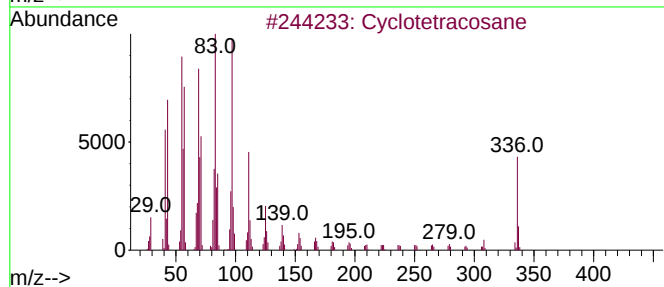
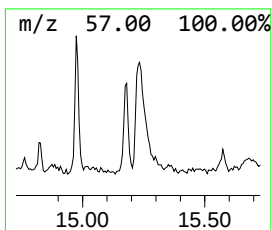
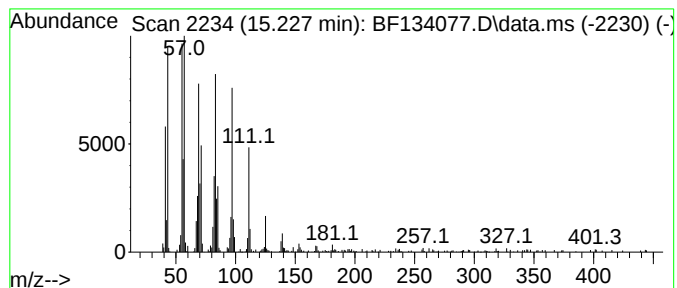
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Tetracosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.227	19.11 ng	562201	Perylene-d12		15.545	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclotetracosane		336	C24H48	000297-03-0	98
2	1-Tetracosene		336	C24H48	010192-32-2	94
3	Heptacos-1-ene		378	C27H54	015306-27-1	94
4	Trifluoroacetoxy hexadecane		338	C18H33F3O2	006222-03-3	94
5	1-Heneicosanol		312	C21H44O	015594-90-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070523\
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Acq On : 05 Jul 2023 20:59
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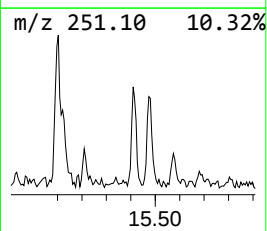
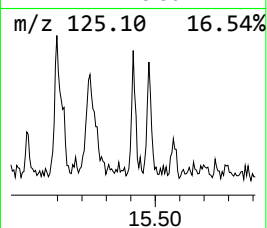
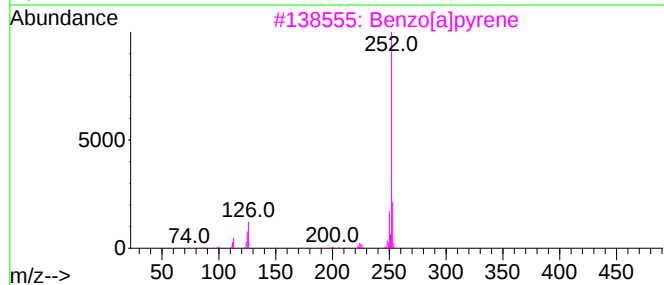
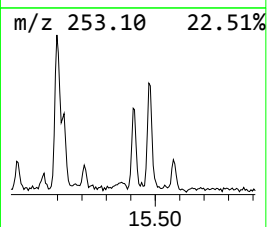
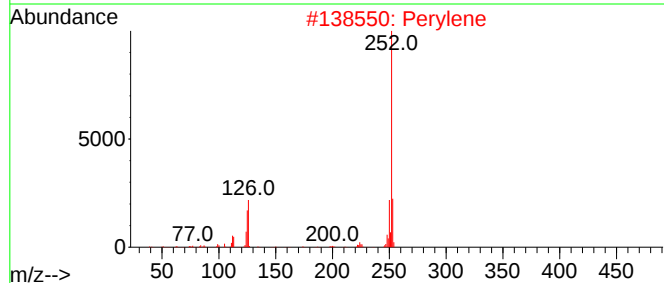
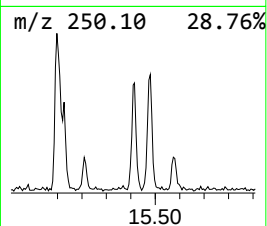
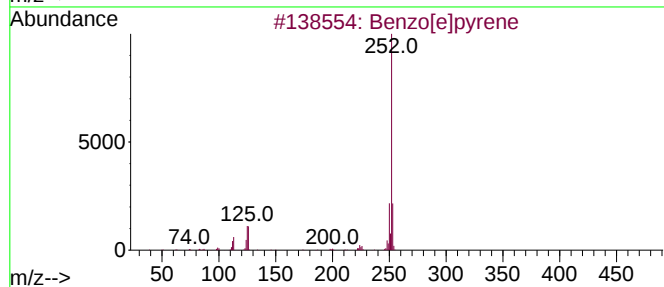
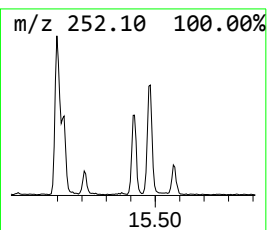
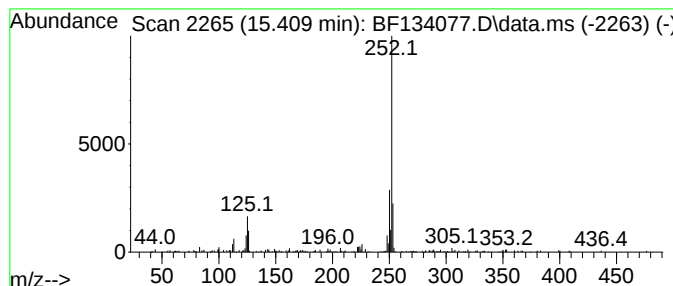
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzo[e]pyrene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.409	3.16 ng	93064	Perylene-d12	15.545

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[e]pyrene	252	C20H12	000192-97-2	96
2		Perylene	252	C20H12	000198-55-0	89
3		Benzo[a]pyrene	252	C20H12	000050-32-8	81
4		Benzo[b]fluoranthene	252	C20H12	000205-99-2	76
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070523\
Data File : BF134077.D
Acq On : 05 Jul 2023 20:59
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ALS Vial : 6 Sample Multiplier: 1

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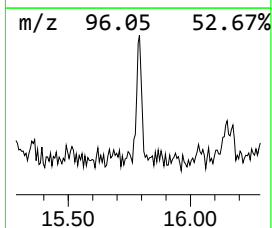
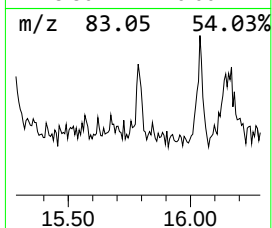
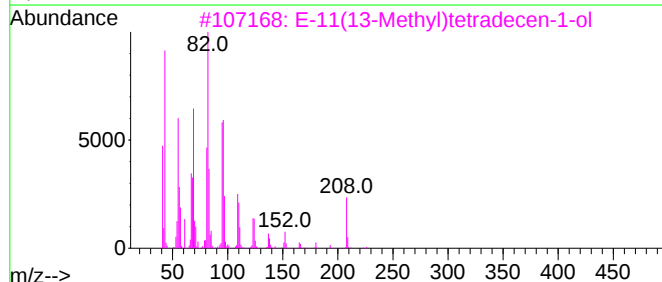
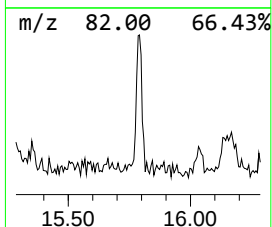
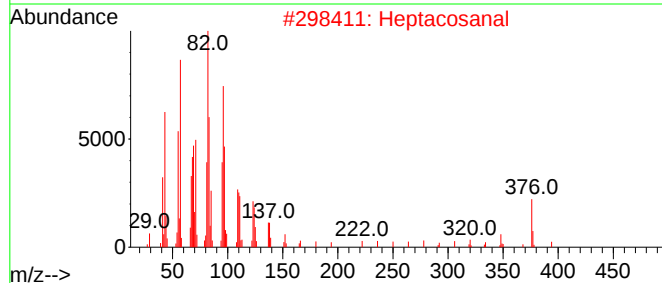
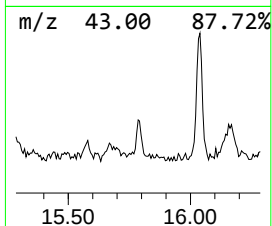
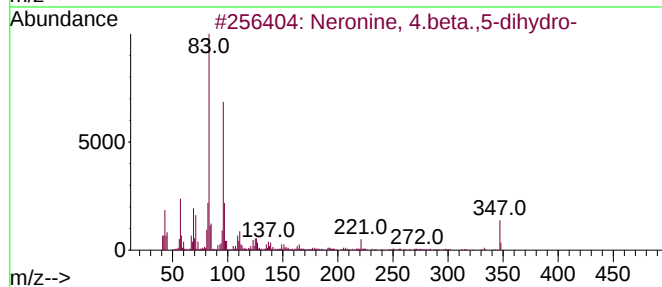
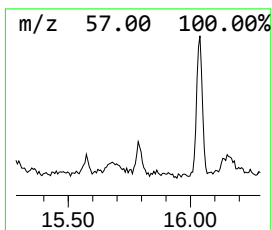
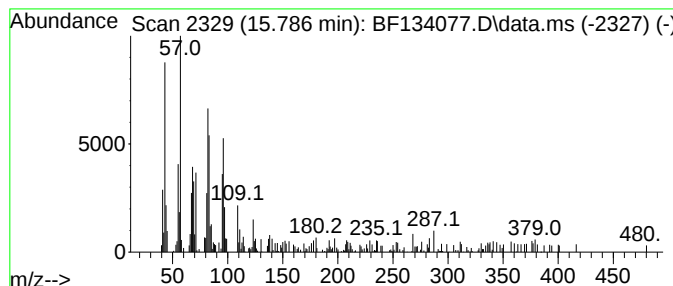
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Nerone, 4.beta.,5-dihydro- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.786	3.58 ng	105213	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nerone, 4.beta.,5-dihydro-	347	C18H21NO6	019483-30-8	64
2			Heptacosanal	394	C27H54O	072934-03-3	62
3			E-11(13-Methyl)tetradecen-1-ol	226	C15H30O	1000130-80-3	58
4			E-11(13-Methyl)tetradecen-1-ol a...	268	C17H32O2	1000130-80-4	58
5			13-Methyl-12-tetradecen-1-ol ace...	268	C17H32O2	099798-78-4	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070523\
Data File : BF134077.D
Acq On : 05 Jul 2023 20:59
Operator : CG\JU
Sample : 03483-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

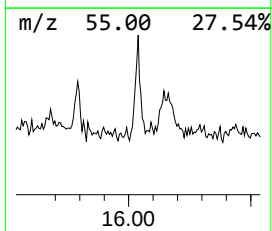
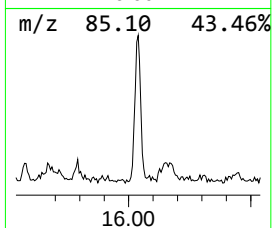
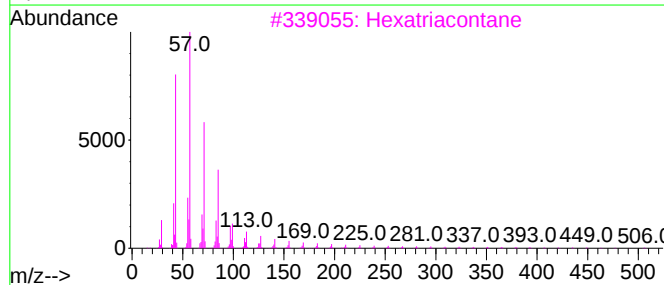
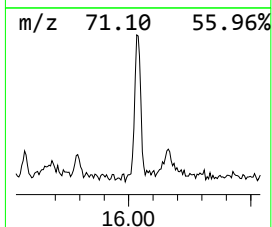
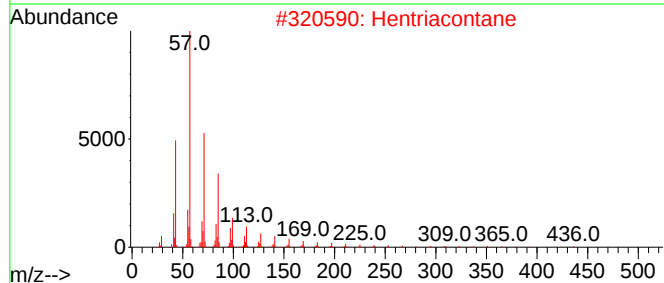
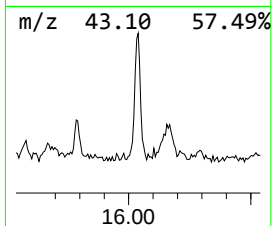
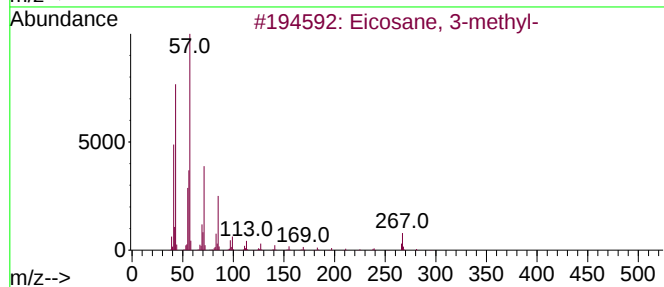
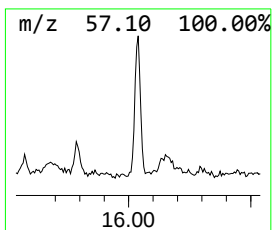
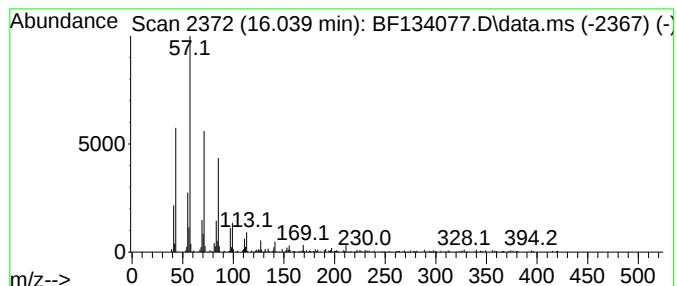
Instrument :
BNA_F
ClientSampleId :
RO-CHRT-24801

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 13 Eicosane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.039	7.82 ng	230189	Perylene-d12	15.545	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 3-methyl-	296	C21H44	006418-46-8	93
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Hexatriacontane	507	C36H74	000630-06-8	91
4	Octacosane	394	C28H58	000630-02-4	89
5	Tetratetracontane	619	C44H90	007098-22-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070523\
Data File : BF134077.D
Acq On : 05 Jul 2023 20:59
Operator : CG\JU
Sample : 03483-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-CHRT-24801

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...	2.175	34.8	ng	1416990	1	6.845	814099	20.0
2-Pentanone, 4-...	5.104	4.5	ng	183478	1	6.845	814099	20.0
Benzophenone	10.598	8.2	ng	445437	3	9.886	1088510	20.0
n-Hexadecanoic ...	11.910	15.5	ng	802141	4	11.380	1036540	20.0
Octadecanoic acid	12.704	16.3	ng	842375	4	11.380	1036540	20.0
Cycloeicosane	13.898	7.6	ng	391154	5	14.039	1031860	20.0
Cyclotetracosane	14.545	6.2	ng	321644	5	14.039	1031860	20.0
Docosanal	14.974	10.1	ng	298150	6	15.545	588465	20.0
Heptacosane	15.180	3.6	ng	105674	6	15.545	588465	20.0
1-Tetracosene	15.227	19.1	ng	562201	6	15.545	588465	20.0
Benzo[e]pyrene	15.409	3.2	ng	93064	6	15.545	588465	20.0
Neronine, 4.bet...	15.786	3.6	ng	105213	6	15.545	588465	20.0
Eicosane, 3-met...	16.039	7.8	ng	230189	6	15.545	588465	20.0