

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
 Data File : BF131592.D
 Acq On : 12 Dec 2022 14:54
 Operator : CG\JU
 Sample : N5964-09
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SU-518-COMP-05

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-BF120822.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131592.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	6	14	21	rVB	462293	598374	32.75%	4.648%
2	2.275	27	32	41	rBV	21004	27663	1.51%	0.215%
3	5.110	508	514	523	rVB	203859	272109	14.89%	2.114%
4	5.516	578	583	586	rBV	1489957	1515728	82.95%	11.775%
5	6.528	749	755	758	rBV	1587190	1558274	85.28%	12.105%
6	6.892	813	817	820	rBV	441921	344359	18.85%	2.675%
7	7.457	908	913	916	rBV	1064867	999241	54.68%	7.762%
8	8.181	1031	1036	1039	rBV	520339	431834	23.63%	3.355%
9	9.263	1215	1220	1223	rBV	2128846	1827288	100.00%	14.195%
10	9.945	1332	1336	1340	rVB	634680	520299	28.47%	4.042%
11	10.739	1467	1471	1475	rBV	1402999	1249418	68.38%	9.706%
12	11.445	1587	1591	1594	rBV	595384	537709	29.43%	4.177%
13	11.510	1598	1602	1605	rVB3	27200	21523	1.18%	0.167%
14	11.969	1674	1680	1683	rBV	72230	85385	4.67%	0.663%
15	13.039	1857	1862	1865	rBV	1993570	1635977	89.53%	12.709%
16	13.263	1888	1900	1907	rBV2	43194	100080	5.48%	0.777%
17	14.027	2020	2030	2038	rBV5	58772	185193	10.13%	1.439%
18	14.098	2038	2042	2045	rVV	379124	331709	18.15%	2.577%
19	14.257	2065	2069	2075	rBV	23320	22247	1.22%	0.173%
20	14.627	2127	2132	2141	rBV3	42133	93505	5.12%	0.726%
21	14.880	2169	2175	2182	rVB4	18255	37146	2.03%	0.289%
22	15.233	2227	2235	2243	rVB2	34187	72197	3.95%	0.561%
23	15.610	2294	2299	2307	rBV	225440	297723	16.29%	2.313%
24	15.921	2343	2352	2358	rBV4	21343	52545	2.88%	0.408%
25	16.704	2478	2485	2494	rBV4	13317	33402	1.83%	0.259%
26	17.092	2548	2551	2558	rVB6	11531	22013	1.20%	0.171%

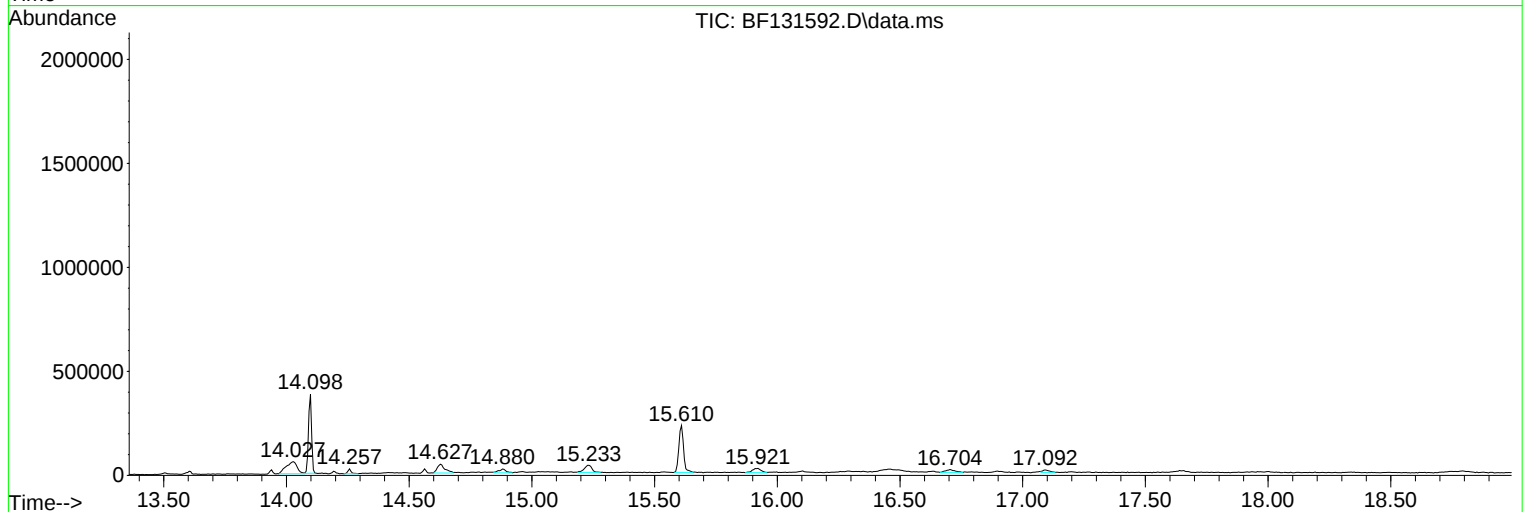
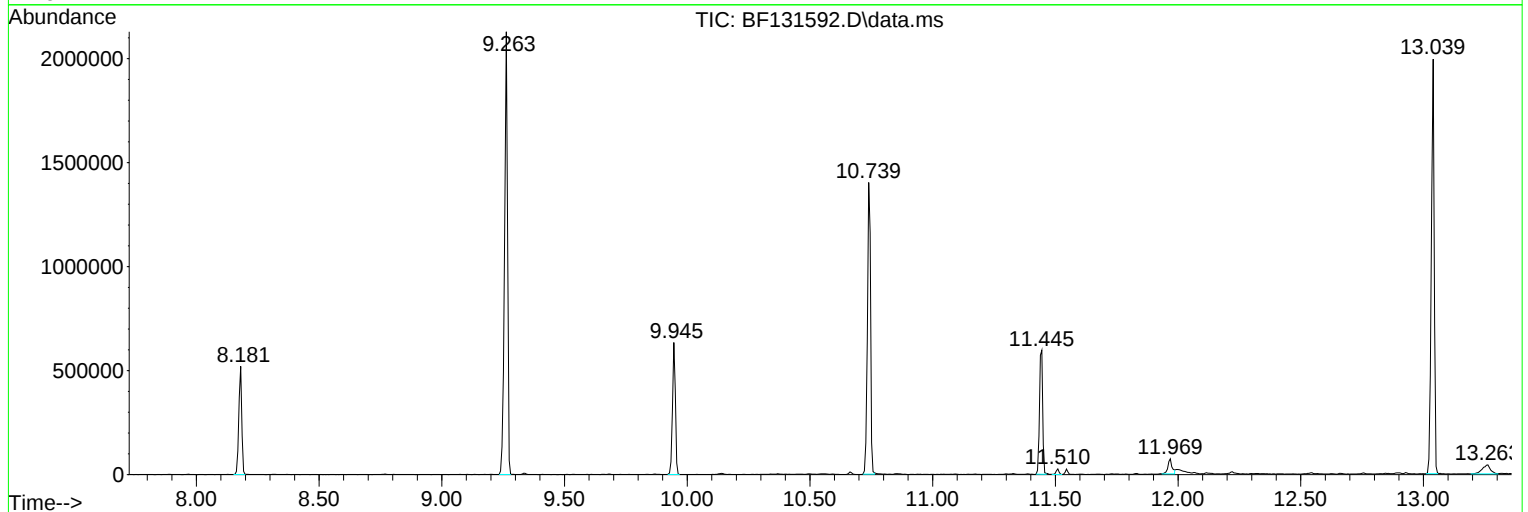
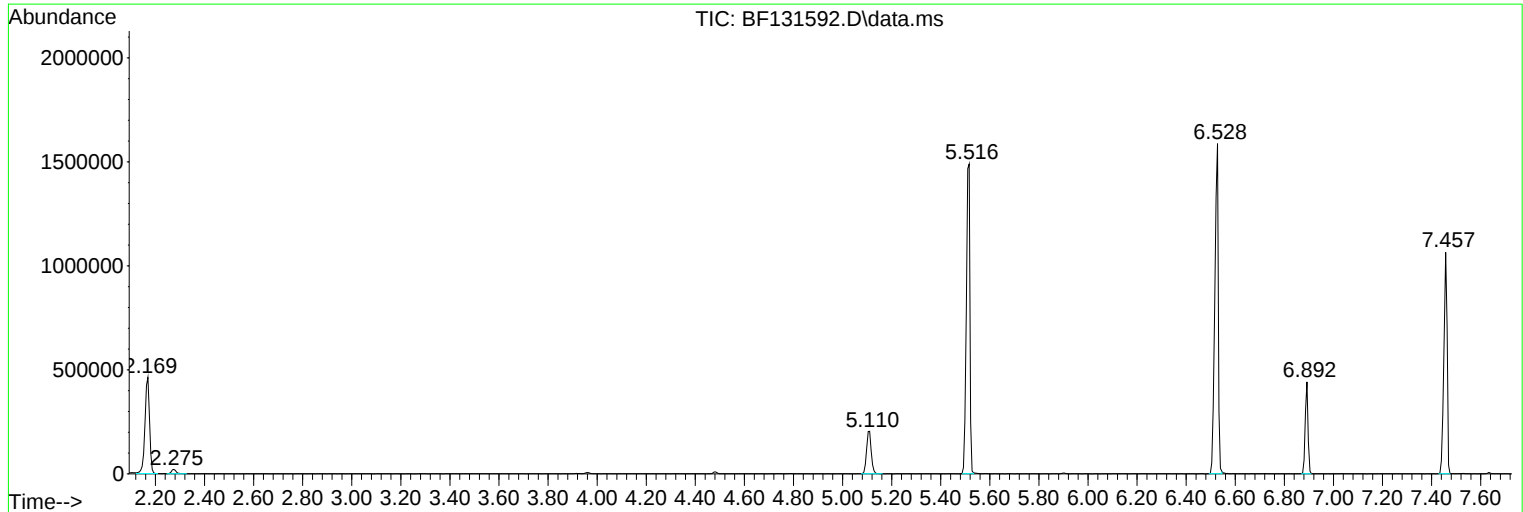
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ClientSampleId :
SU-518-COMP-05

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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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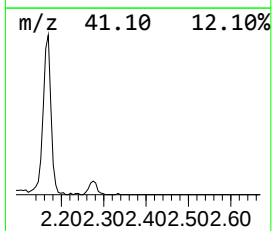
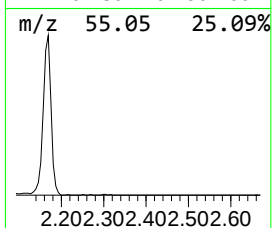
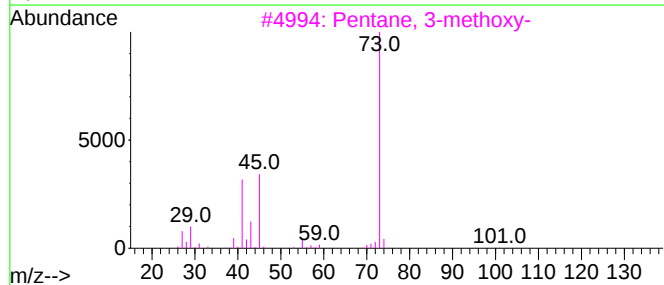
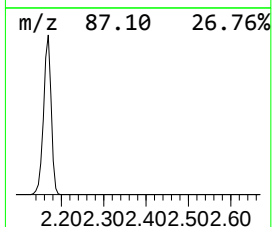
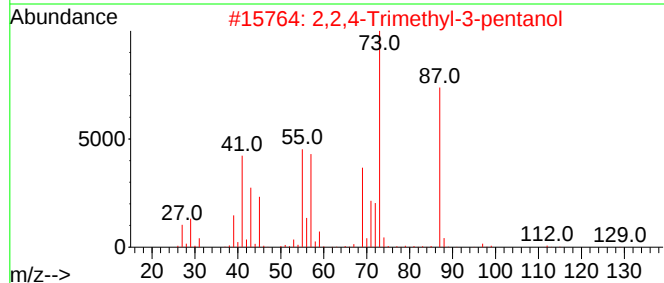
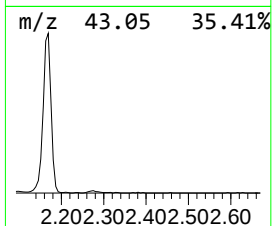
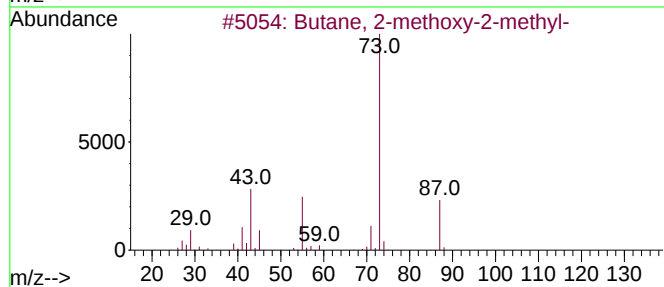
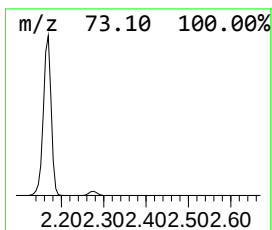
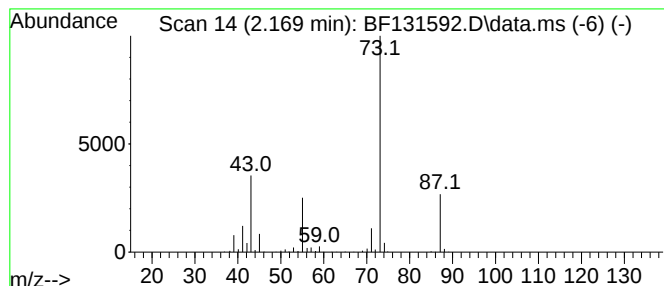
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	34.75 ng	598374	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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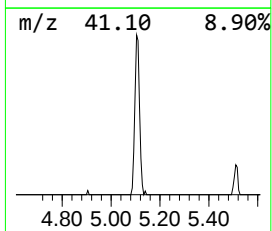
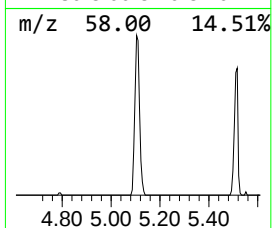
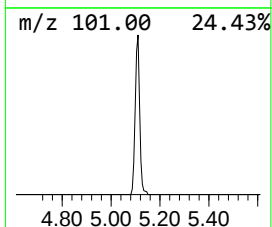
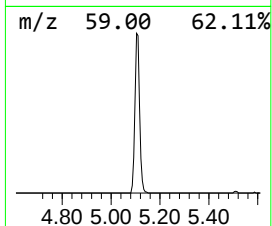
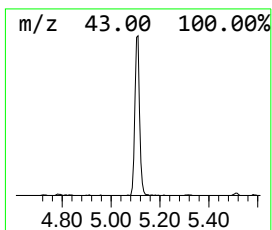
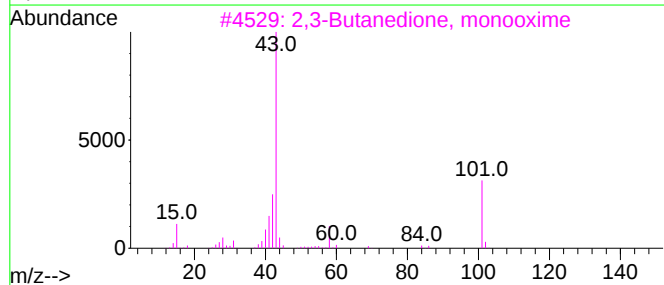
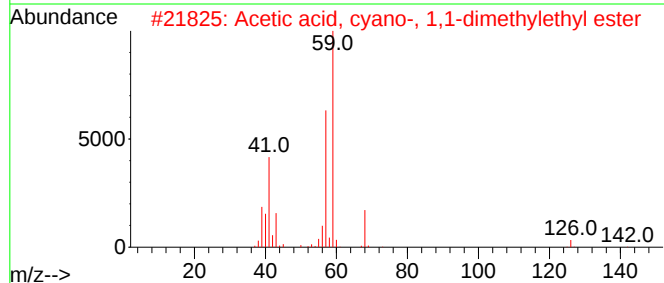
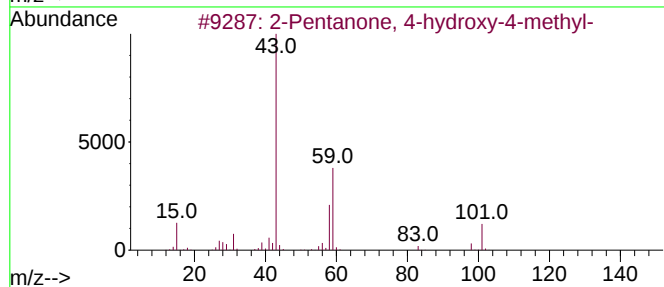
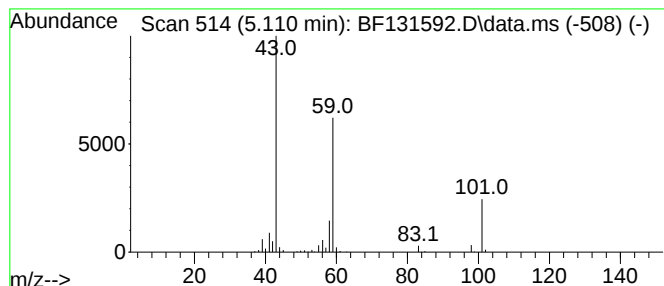
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	15.80 ng	272109	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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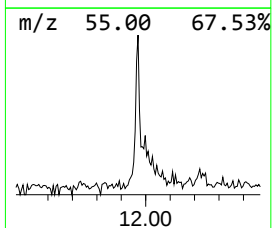
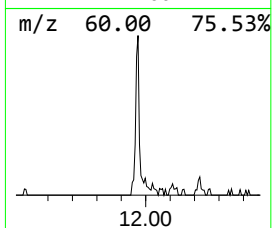
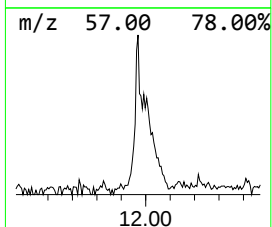
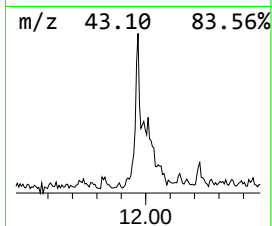
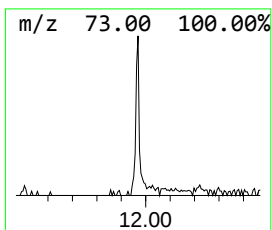
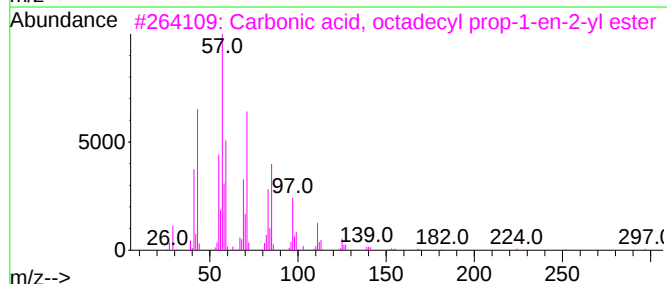
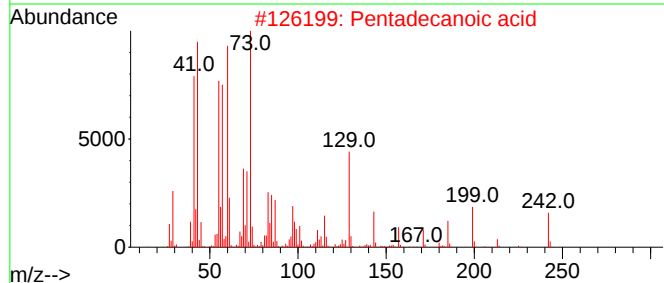
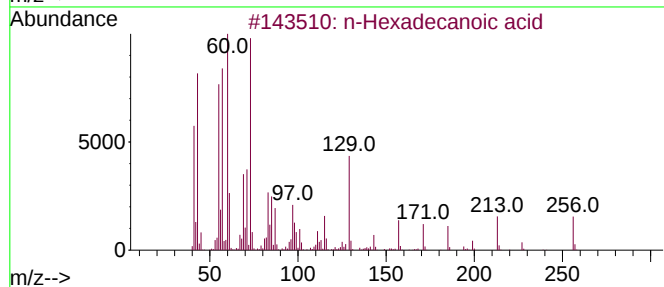
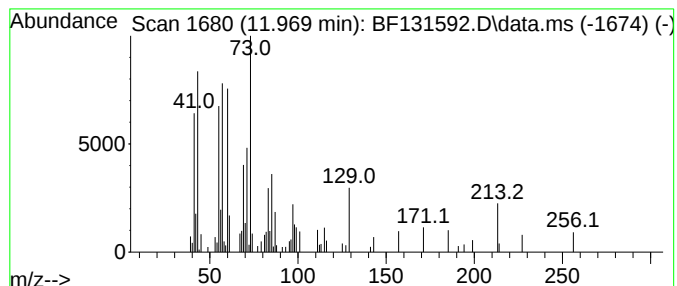
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	3.18 ng	85385	Phenanthrene-d10	11.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	52
3			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	35
4			Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	25
5			Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20



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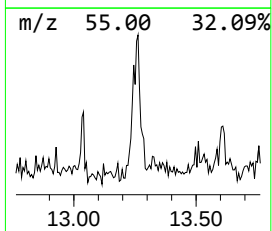
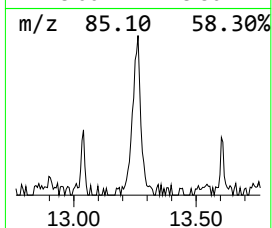
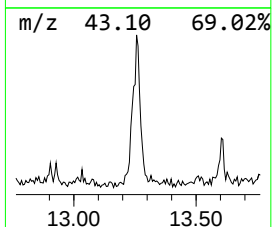
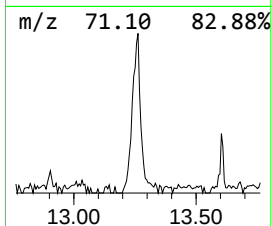
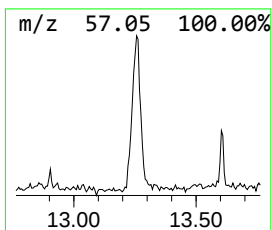
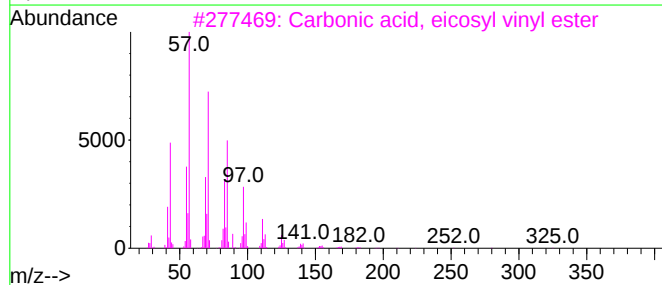
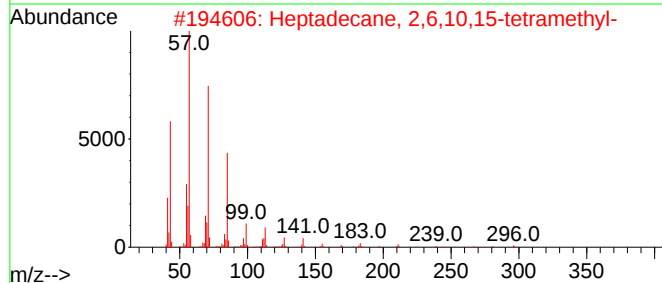
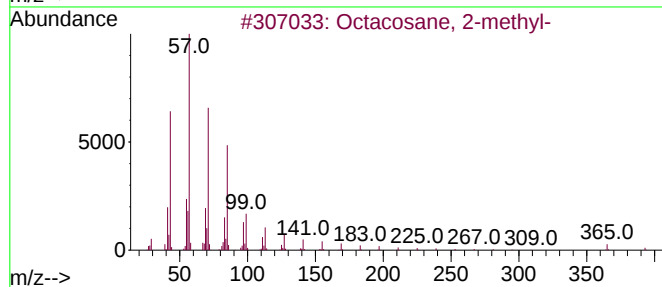
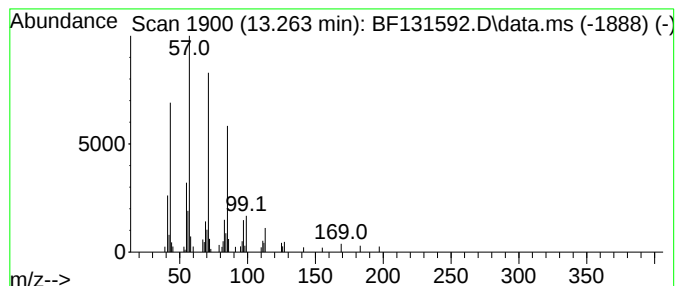
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Peak Number 4 Octacosane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.263	6.03 ng	100080	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
2			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
3			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	86
4			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	83
5			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80



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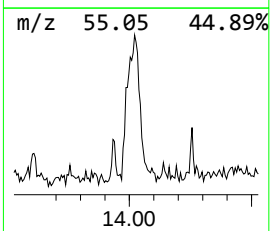
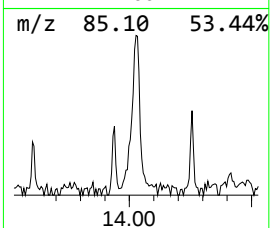
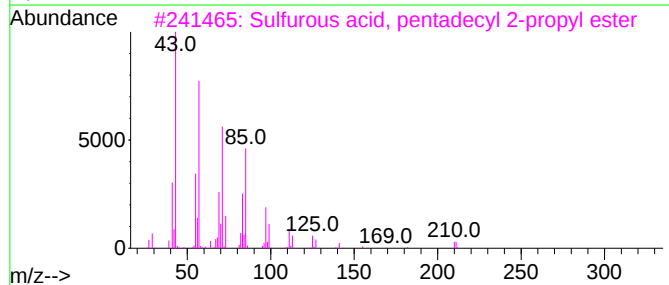
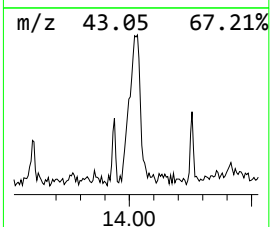
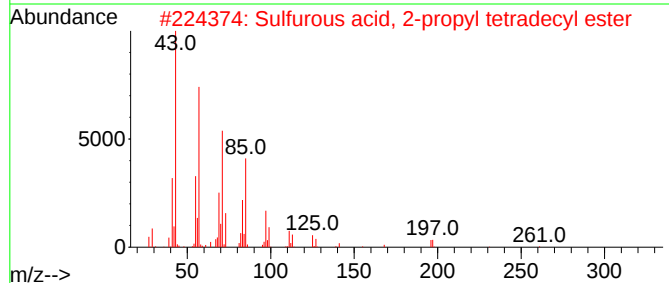
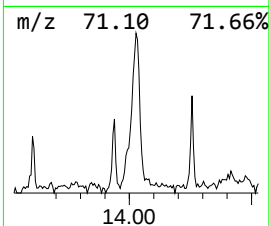
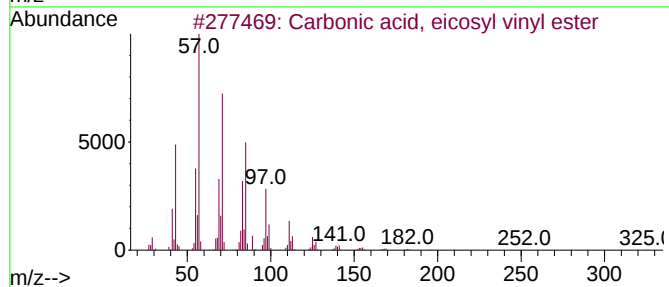
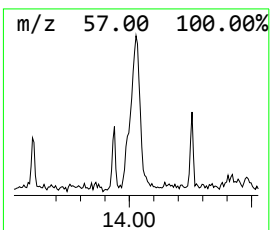
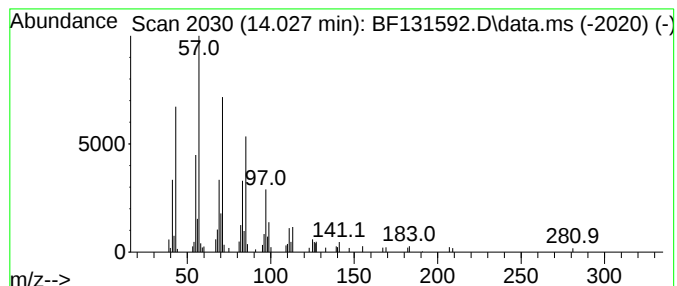
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Peak Number 5 Carbonic acid, eicosyl vinyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.027	11.17 ng	185193	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	91
2			Sulfurous acid, 2-propyl tetradecyl ester	320	C17H36O3S	1010309-12-5	90
3			Sulfurous acid, pentadecyl 2-propyl ester	334	C18H38O3S	1000309-12-6	90
4			Carbonic acid, octadecyl vinyl ester	340	C21H40O3	1000382-54-4	87
5			Sulfurous acid, dodecyl 2-propyl ester	292	C15H32O3S	1000309-12-3	86



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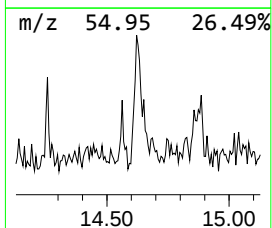
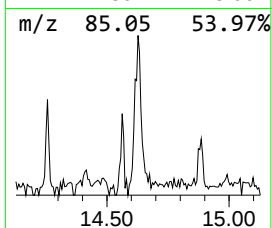
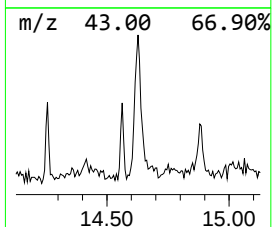
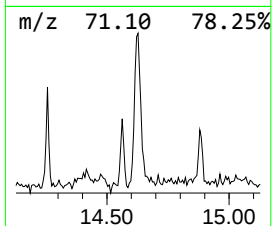
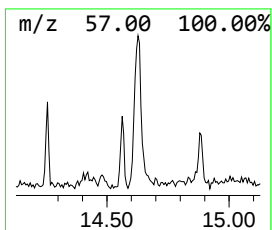
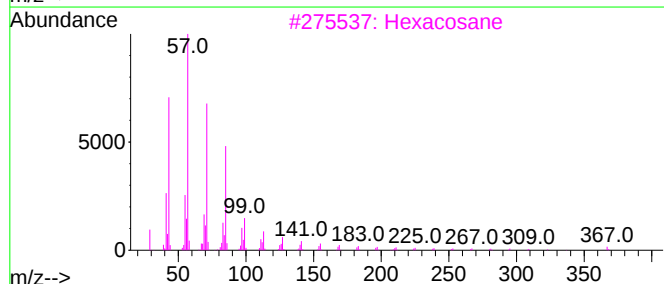
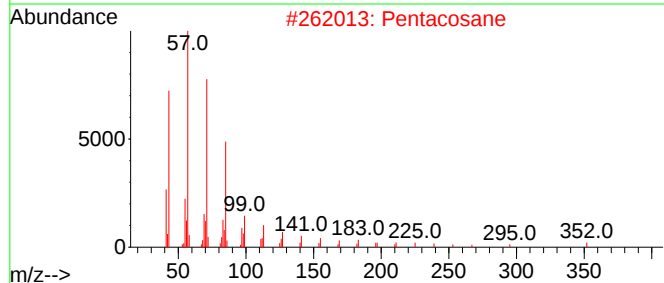
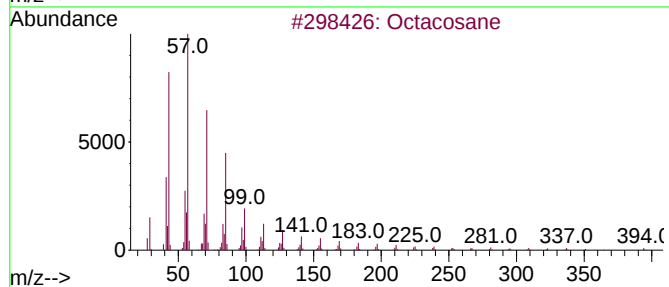
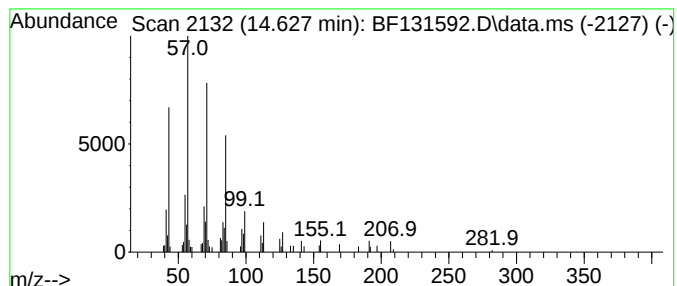
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.627	5.64 ng	93505	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Pentacosane	352	C25H52	000629-99-2	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Heneicosane	296	C21H44	000629-94-7	91
5			Heptadecane	240	C17H36	000629-78-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131592.D
Acq On : 12 Dec 2022 14:54
Operator : CG\JU
Sample : N5964-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-518-COMP-05

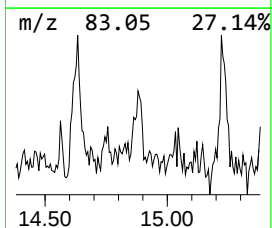
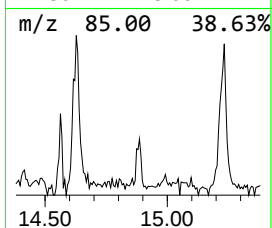
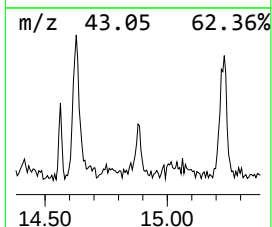
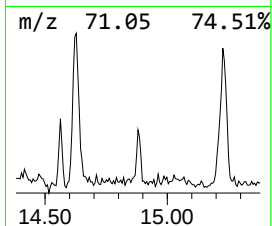
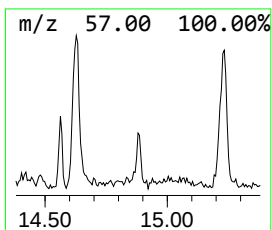
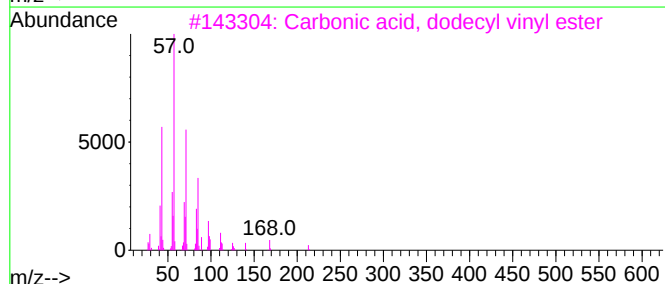
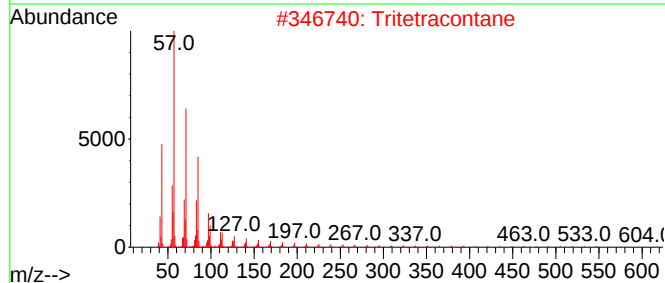
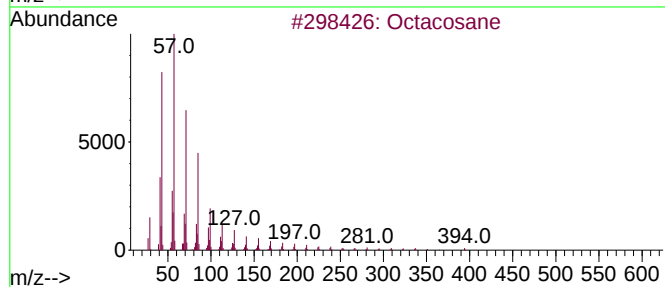
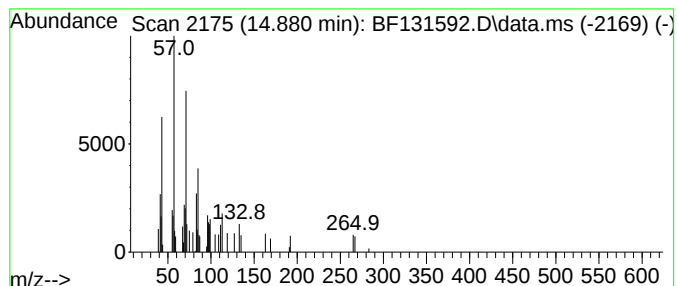
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tritetracontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.880	2.50 ng	37146	Perylene-d12	15.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	72
2			Tritetracontane	605	C43H88	007098-21-7	72
3			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	72
4			Hexacosane	366	C26H54	000630-01-3	64
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131592.D
Acq On : 12 Dec 2022 14:54
Operator : CG\JU
Sample : N5964-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-518-COMP-05

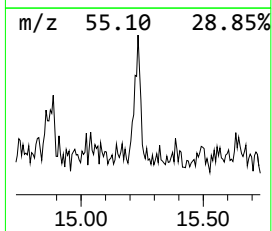
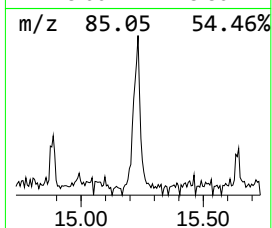
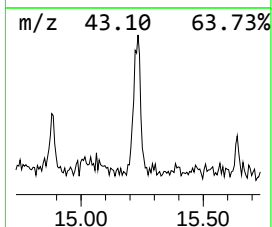
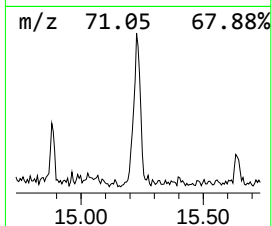
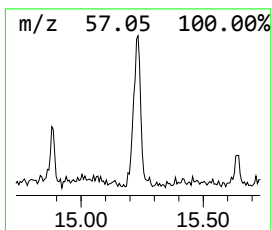
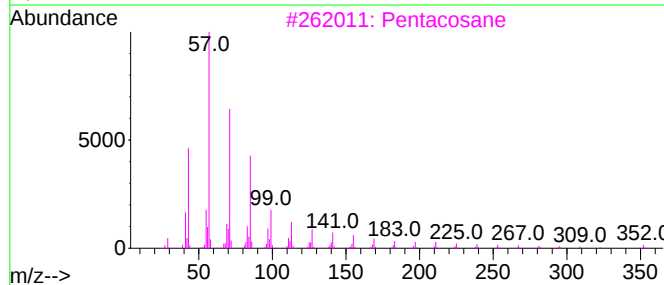
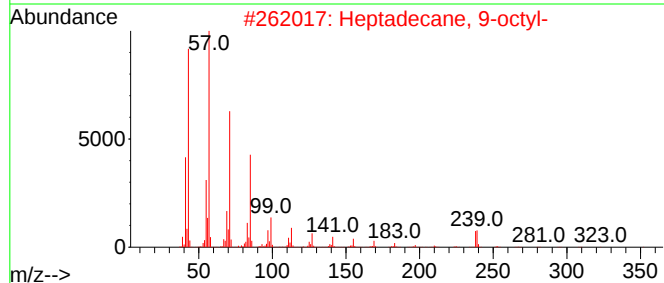
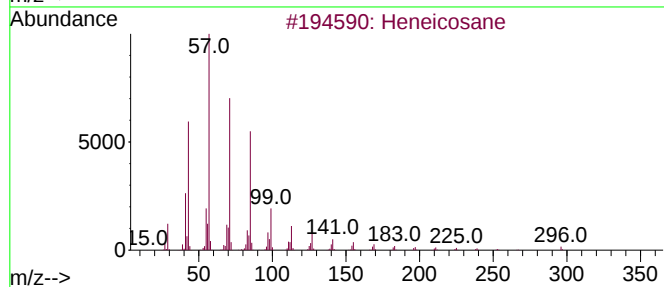
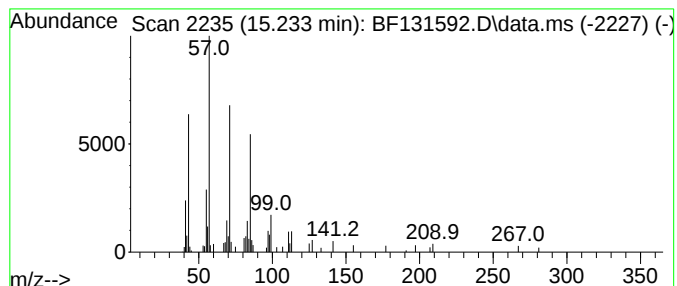
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.233	4.85 ng	72197	Perylene-d12	15.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	87
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
3			Pentacosane	352	C25H52	000629-99-2	83
4			Octadecane	254	C18H38	000593-45-3	80
5			Nonadecane	268	C19H40	000629-92-5	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131592.D
Acq On : 12 Dec 2022 14:54
Operator : CG\JU
Sample : N5964-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-518-COMP-05

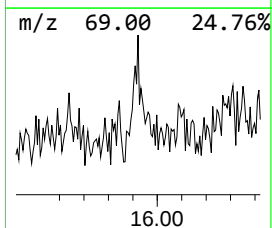
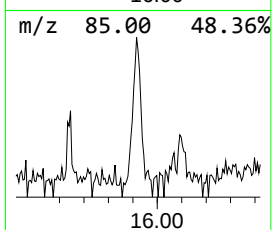
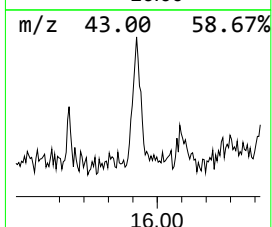
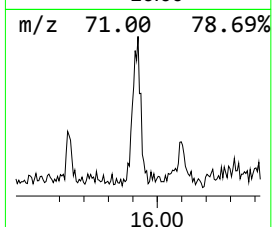
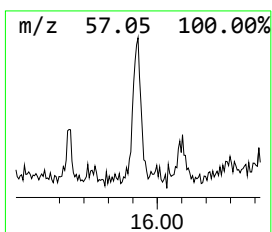
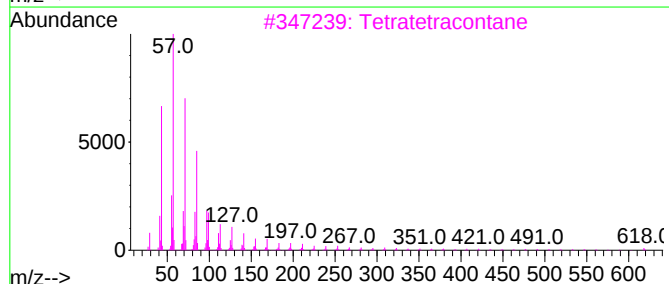
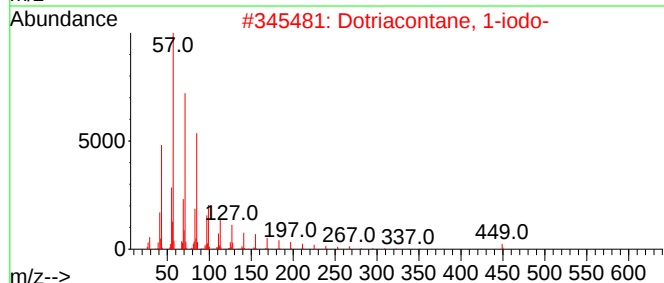
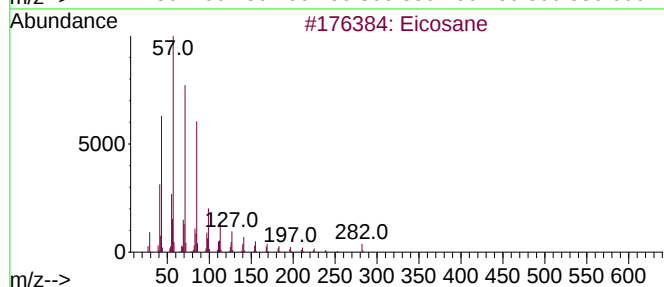
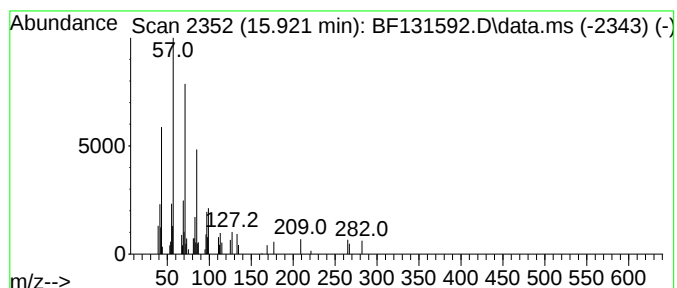
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	3.53 ng	52545	Perylene-d12	15.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	81
2			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	72
3			Tetratetracontane	619	C44H90	007098-22-8	72
4			Heneicosane	296	C21H44	000629-94-7	64
5			Octadecane	254	C18H38	000593-45-3	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
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Acq On : 12 Dec 2022 14:54
Operator : CG\JU
Sample : N5964-09
Misc :
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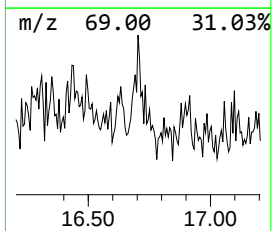
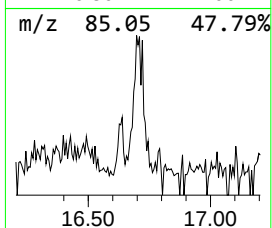
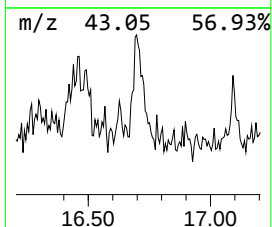
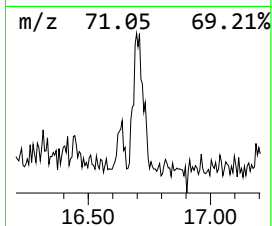
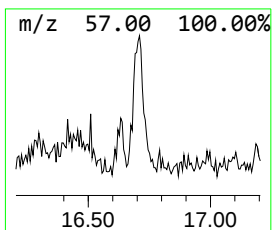
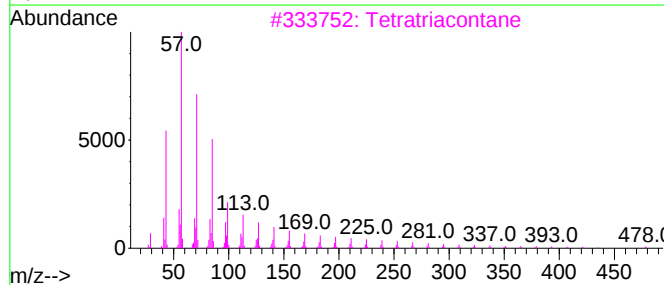
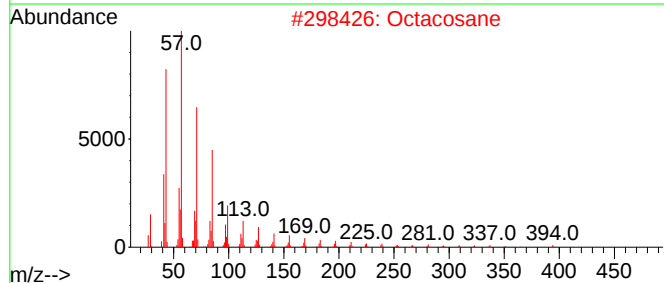
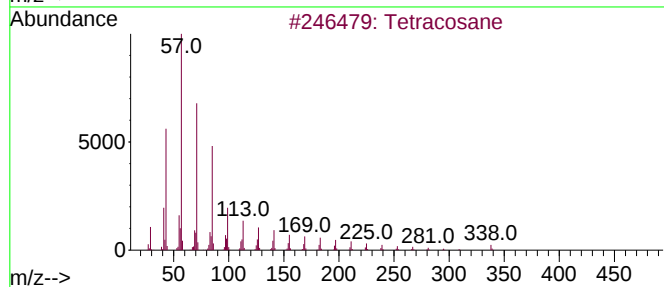
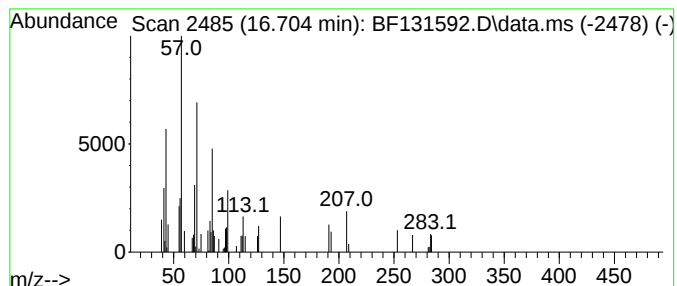
Instrument :
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ClientSampleId :
SU-518-COMP-05

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.704	2.24 ng	33402	Perylene-d12	15.610	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	52
2	Octacosane	394	C28H58	000630-02-4	52
3	Tetratriacontane	479	C34H70	014167-59-0	50
4	Hexacosane	366	C26H54	000630-01-3	49
5	Eicosane	282	C20H42	000112-95-8	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131592.D
Acq On : 12 Dec 2022 14:54
Operator : CG\JU
Sample : N5964-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-518-COMP-05

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-...	5.110	15.8	ng	272109	1	6.892	344359	20.0
n-Hexadecanoic ...	11.969	3.2	ng	85385	4	11.445	537709	20.0
Octacosane, 2-m...	13.263	6.0	ng	100080	5	14.098	331709	20.0
Carbonic acid, ...	14.027	11.2	ng	185193	5	14.098	331709	20.0
Octacosane	14.627	5.6	ng	93505	5	14.098	331709	20.0
Tritetracontane	14.880	2.5	ng	37146	6	15.610	297723	20.0
Heneicosane	15.233	4.8	ng	72197	6	15.610	297723	20.0
Eicosane	15.921	3.5	ng	52545	6	15.610	297723	20.0
Tetracosane	16.704	2.2	ng	33402	6	15.610	297723	20.0