

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
 Data File : BF134371.D
 Acq On : 19 Jul 2023 21:57
 Operator : CG\JU
 Sample : 03639-21
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP5

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: BF134371.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	10	19	rVB	280292	377393	18.22%	2.911%
2	5.098	507	512	521	rBV	31750	47455	2.29%	0.366%
3	5.481	573	577	592	rBV	1907164	1784448	86.16%	13.763%
4	6.481	742	747	750	rBV	1788511	1781447	86.02%	13.740%
5	6.834	804	807	813	rBV	437397	397197	19.18%	3.064%
6	7.404	899	904	907	rBV	1179968	1116790	53.92%	8.614%
7	8.116	1021	1025	1028	rBV	631625	490749	23.70%	3.785%
8	9.192	1204	1208	1211	rBV	2667973	2071051	100.00%	15.974%
9	9.875	1320	1324	1327	rBV	566153	497515	24.02%	3.837%
10	10.669	1455	1459	1462	rBV	1420047	1184900	57.21%	9.139%
11	11.369	1574	1578	1581	rBV	517966	441410	21.31%	3.405%
12	11.898	1665	1668	1672	rBV	137796	146565	7.08%	1.130%
13	12.592	1782	1786	1788	rBV	31948	31033	1.50%	0.239%
14	12.686	1799	1802	1812	rBV2	25545	33991	1.64%	0.262%
15	12.821	1820	1825	1829	rVB	24542	26255	1.27%	0.202%
16	12.963	1845	1849	1853	rBV	1819911	1654220	79.87%	12.759%
17	13.639	1961	1964	1968	rBV	80780	73564	3.55%	0.567%
18	13.904	2005	2009	2017	rVB3	39605	87473	4.22%	0.675%
19	14.027	2027	2030	2034	rBV	393161	364390	17.59%	2.810%
20	15.157	2218	2222	2226	rVB2	25430	32109	1.55%	0.248%
21	15.533	2281	2286	2294	rBV	213916	291886	14.09%	2.251%
22	16.009	2363	2367	2373	rVB4	20788	33593	1.62%	0.259%

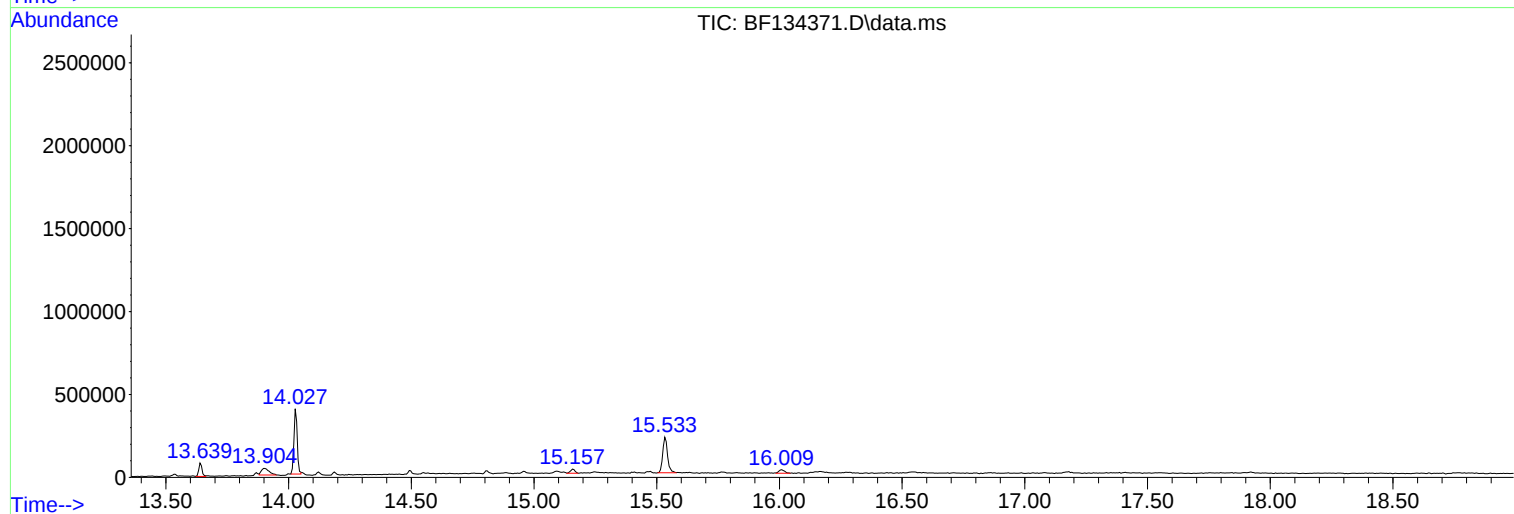
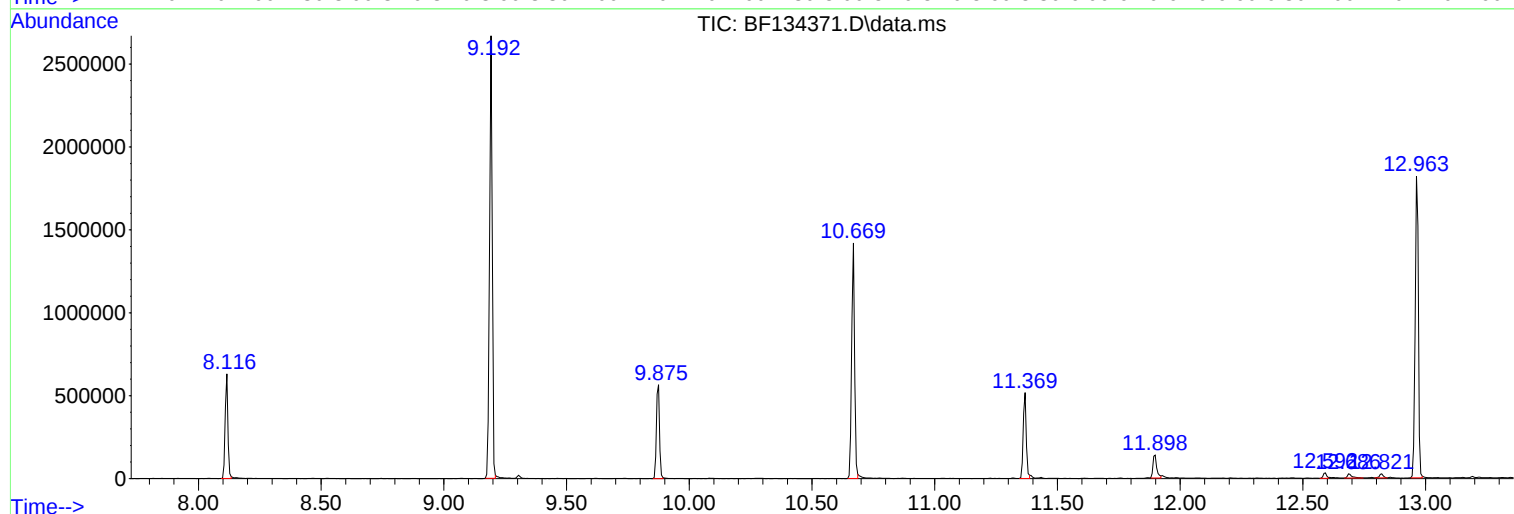
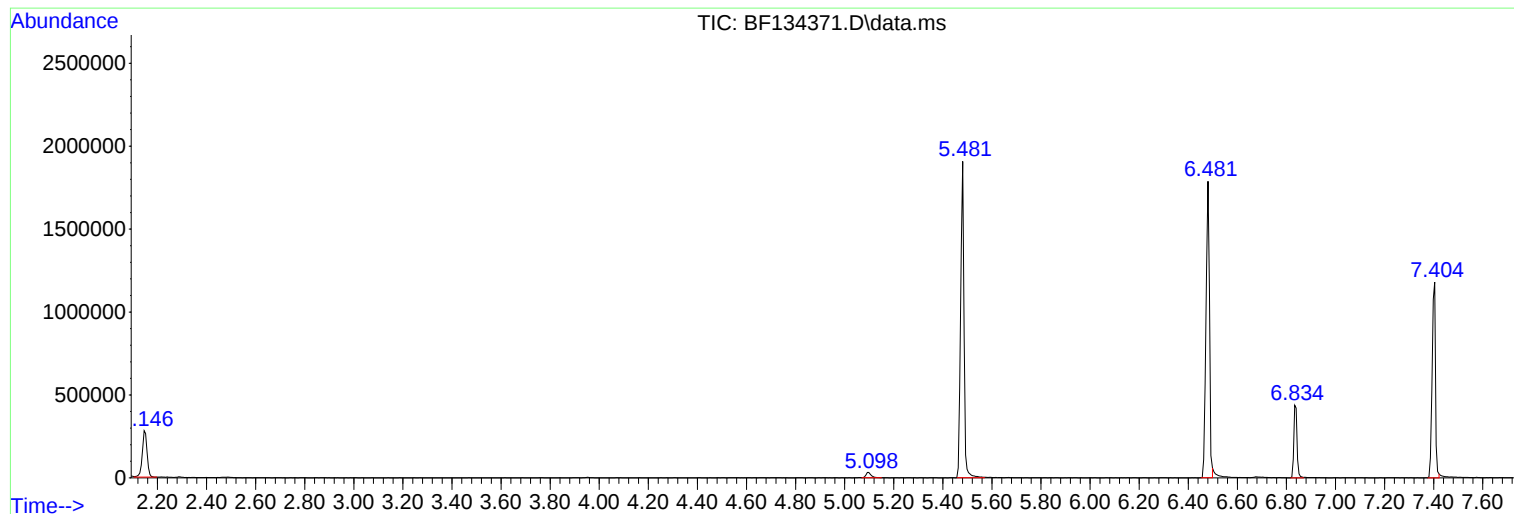
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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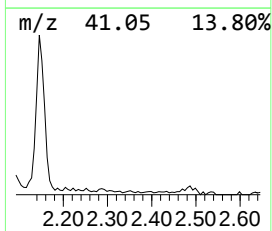
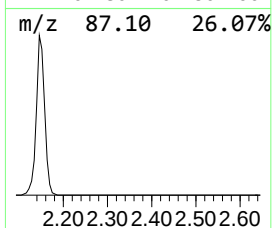
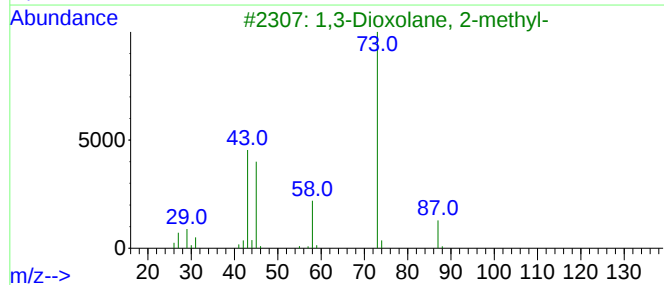
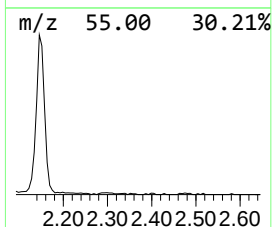
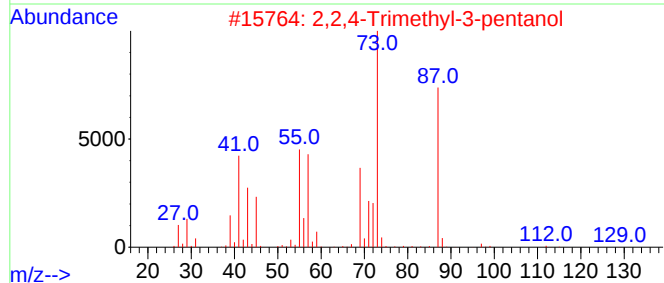
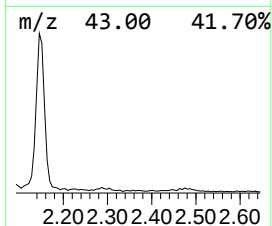
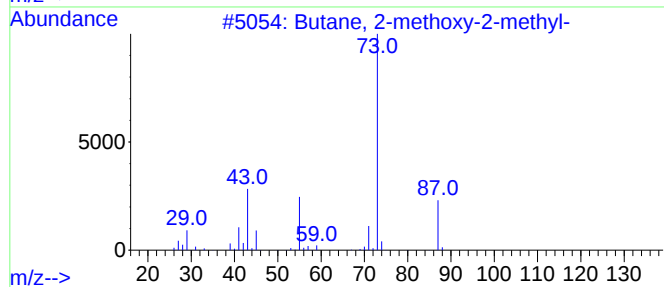
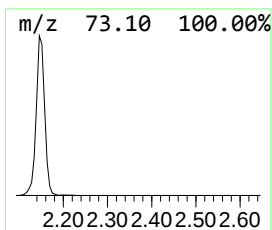
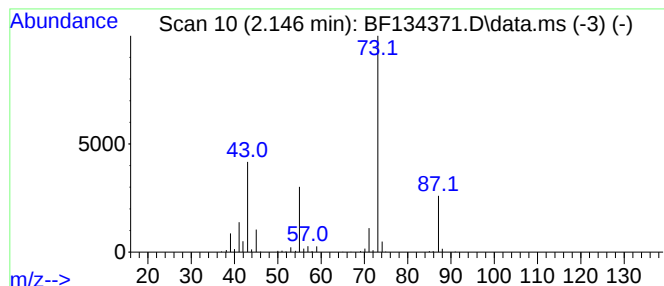
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.146	19.00 ng	377393	1,4-Dichlorobenzene-d4	6.839

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	38
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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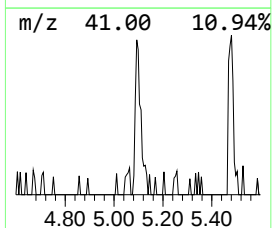
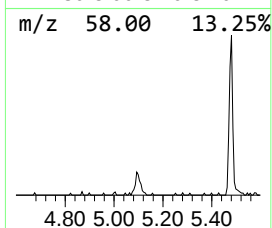
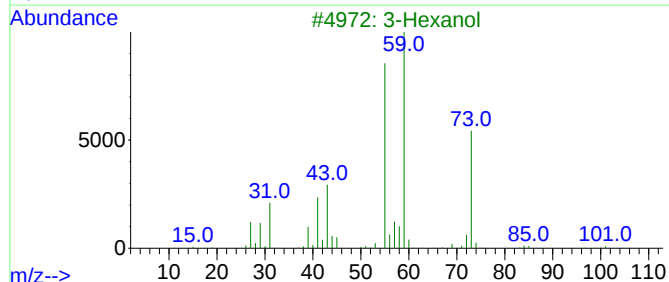
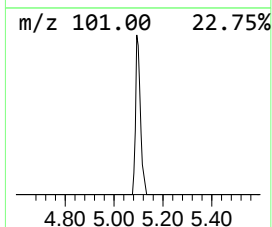
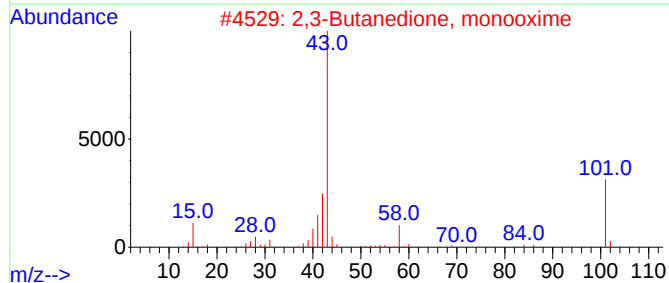
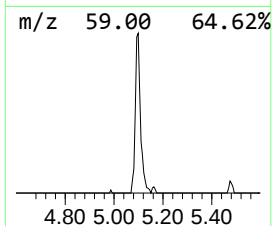
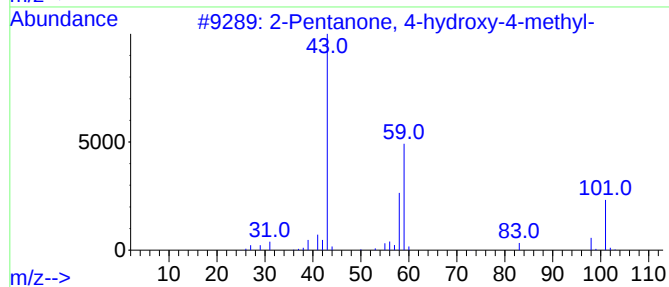
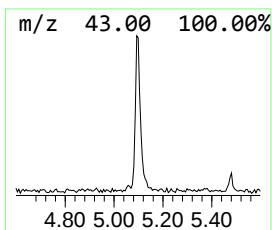
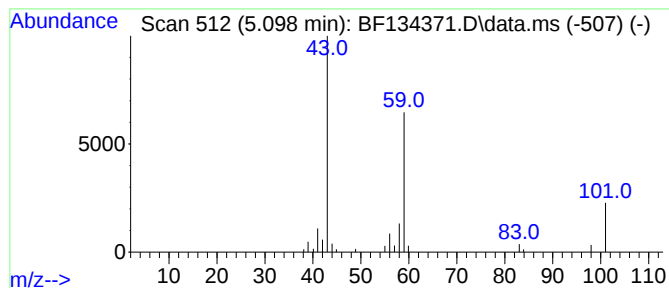
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	2.39 ng	47455	1,4-Dichlorobenzene-d4	6.839

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3		3-Hexanol	102	C6H14O	000623-37-0	25
4		1,2-Butanediol	90	C4H10O2	000584-03-2	23
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	16



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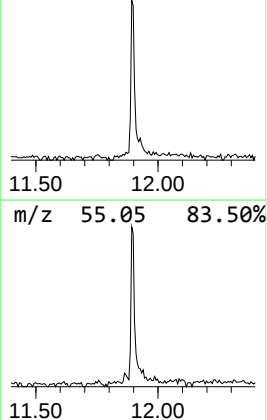
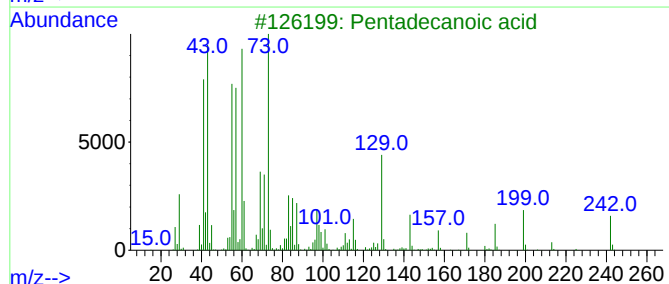
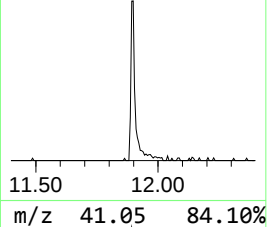
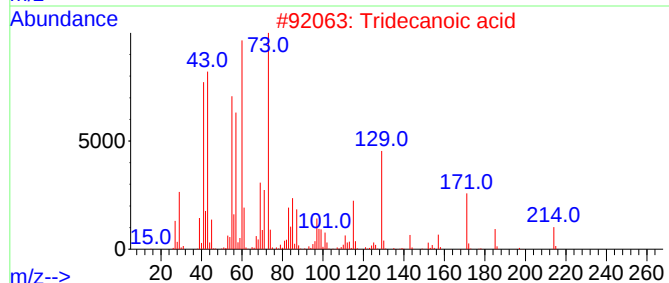
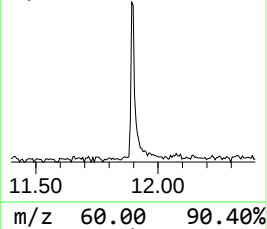
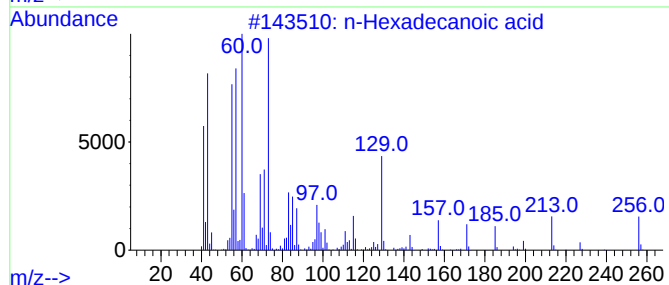
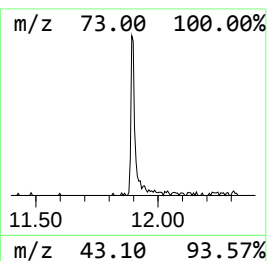
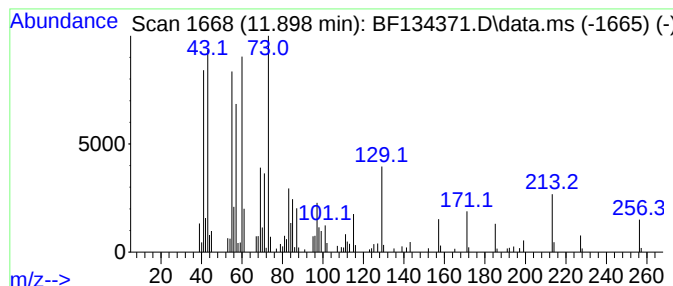
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.898	6.64 ng	146565	Phenanthrene-d10	11.369	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64



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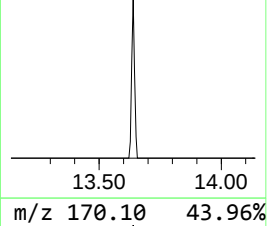
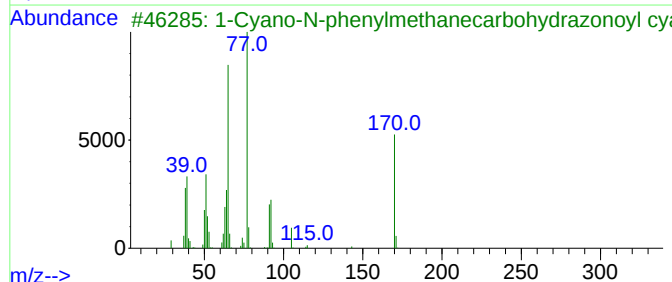
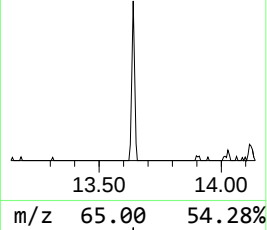
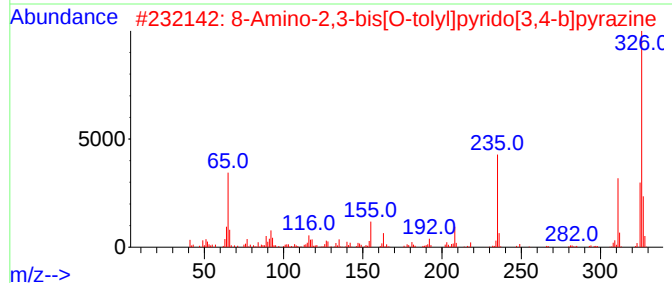
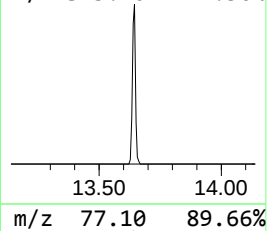
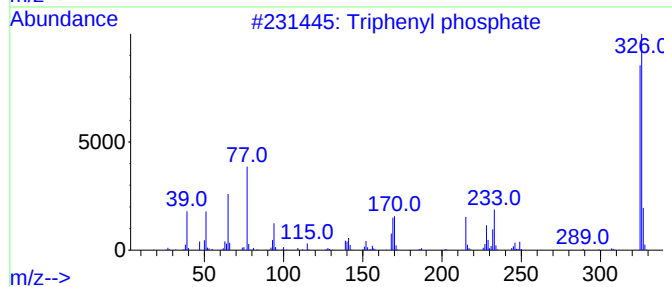
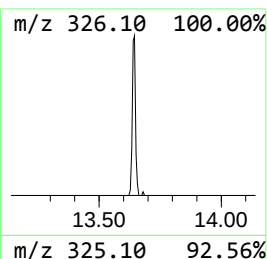
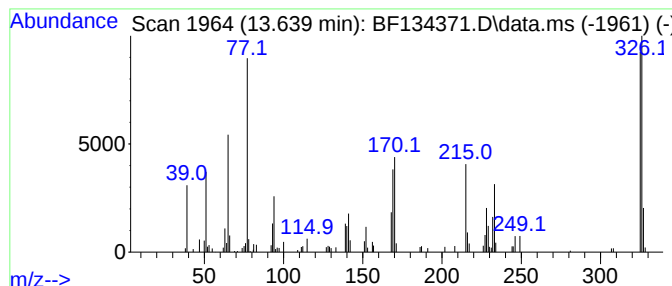
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Peak Number 4 Triphenyl phosphate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.639	4.04 ng	73564	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenyl phosphate	326	C18H15O4P	000115-86-6	99
2			8-Amino-2,3-bis[O-tolyl]pyrido[3...	326	C21H18N4	030146-44-2	32
3			1-Cyano-N-phenylmethanecarbohydr...	170	C9H6N4	000306-18-3	27
4			Demethoxykanugin	326	C18H14O6	001668-33-3	14
5			(1-Allyl-2-oxo-1,2-dihydro-indol...	326	C20H14N4O	1000296-28-1	14



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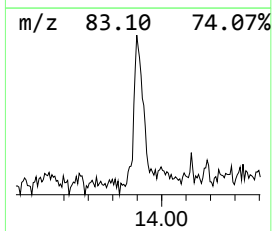
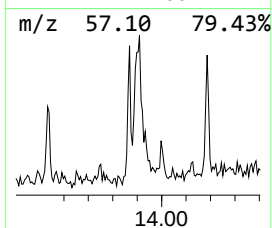
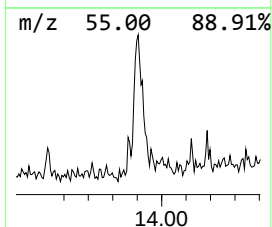
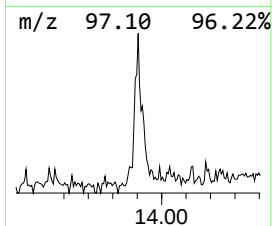
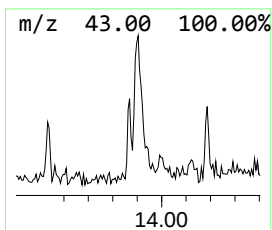
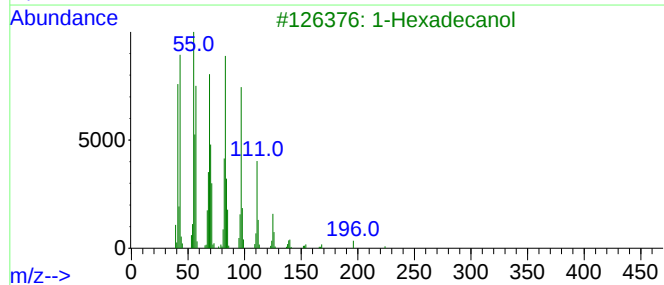
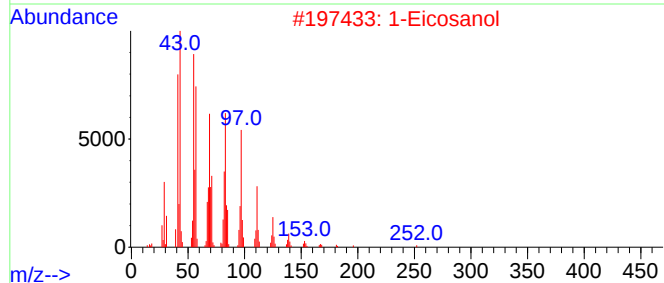
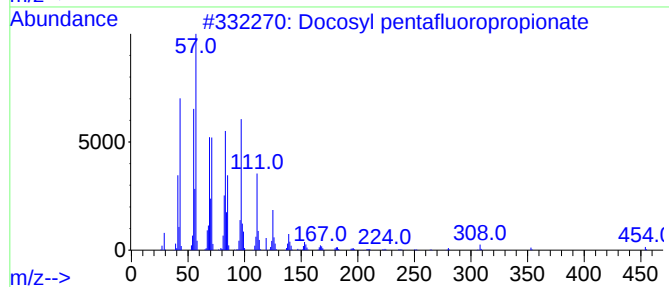
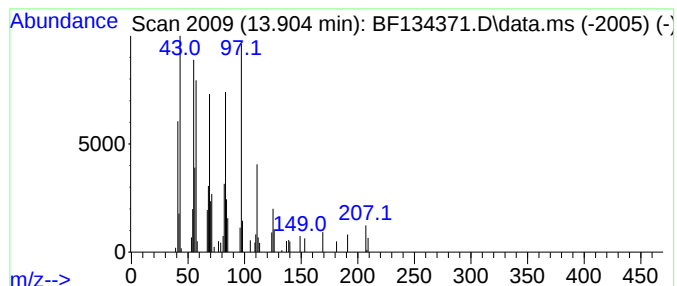
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Docosyl pentafluoropropionate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	4.80 ng	87473	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	86
2			1-Eicosanol	298	C20H42O	000629-96-9	68
3			1-Hexadecanol	242	C16H34O	036653-82-4	64
4			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	64
5			9-Eicosene, (E)-	280	C20H40	074685-29-3	52



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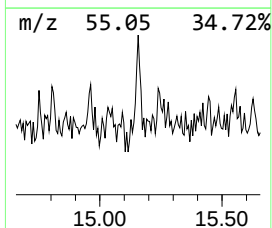
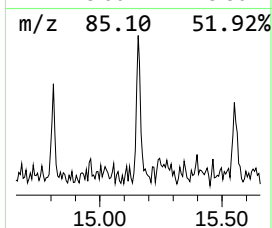
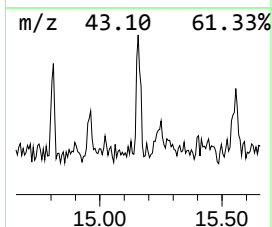
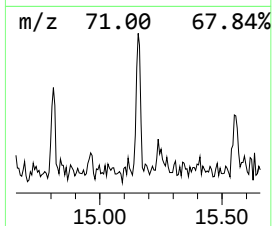
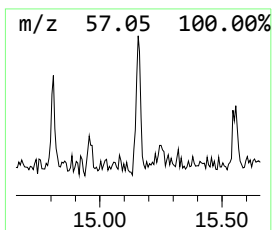
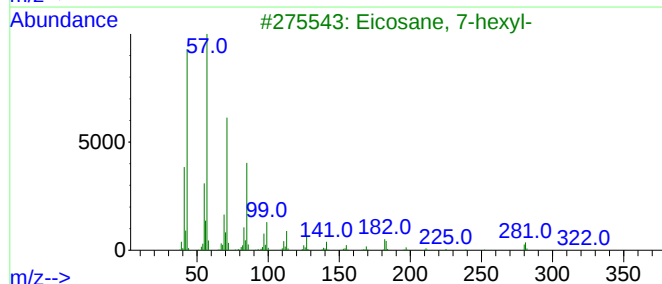
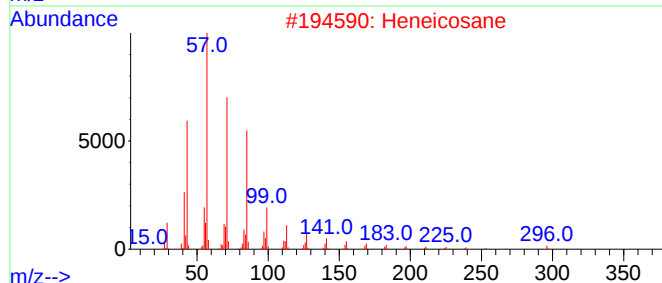
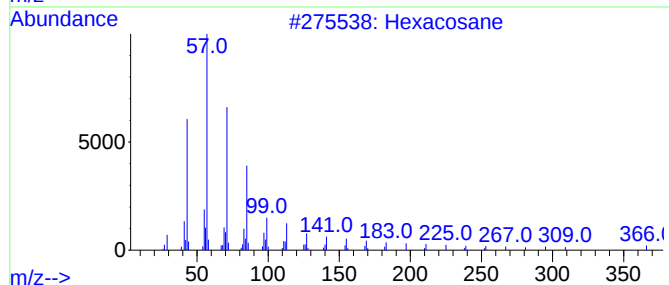
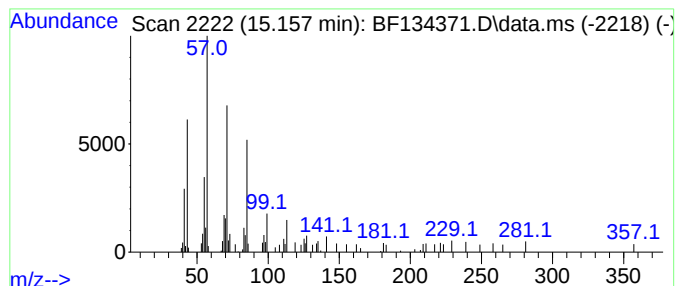
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.157	2.20 ng	32109	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	87
2			Heneicosane	296	C21H44	000629-94-7	81
3			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	80
4			Tetracosane	338	C24H50	000646-31-1	74
5			Octadecane	254	C18H38	000593-45-3	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134371.D
Acq On : 19 Jul 2023 21:57
Operator : CG\JU
Sample : 03639-21
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP5

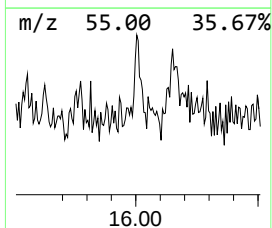
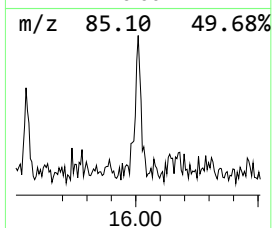
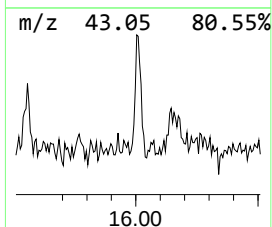
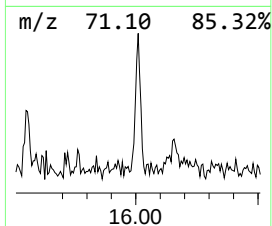
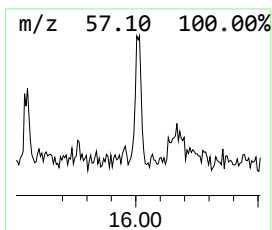
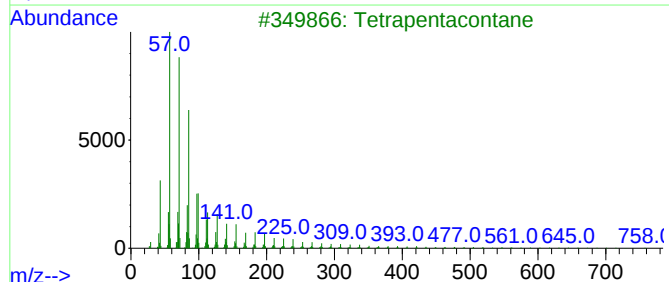
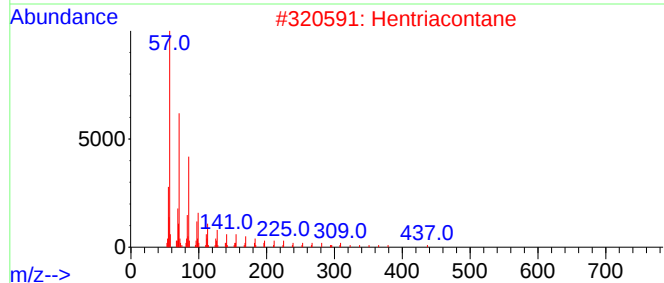
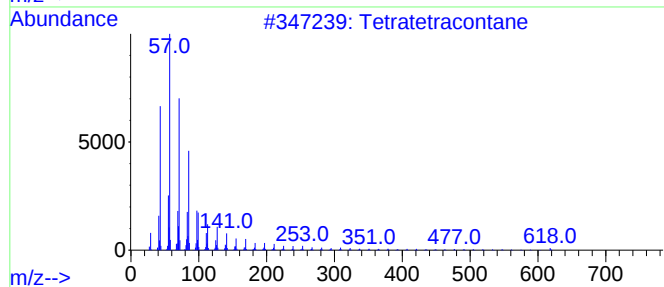
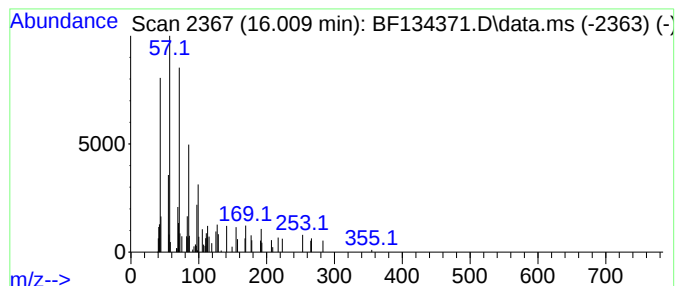
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.009	2.30 ng	33593	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	72
2			Hentriacontane	437	C31H64	000630-04-6	68
3			Tetrapentacontane	759	C54H110	005856-66-6	64
4			Nonadecane, 2,3-dimethyl-	296	C21H44	075163-99-4	59
5			Heptacosane	380	C27H56	000593-49-7	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134371.D
Acq On : 19 Jul 2023 21:57
Operator : CG\JU
Sample : 03639-21
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP5

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...	2.146	19.0	ng	377393	1	6.839	397197	20.0
2-Pentanone, 4-...	5.098	2.4	ng	47455	1	6.839	397197	20.0
n-Hexadecanoic ...	11.898	6.6	ng	146565	4	11.369	441410	20.0
Triphenyl phosph...	13.639	4.0	ng	73564	5	14.027	364390	20.0
Docosyl pentafl...	13.904	4.8	ng	87473	5	14.027	364390	20.0
Hexacosane	15.157	2.2	ng	32109	6	15.533	291886	20.0
Tetratetracontane	16.009	2.3	ng	33593	6	15.533	291886	20.0