

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112423\
 Data File : BF136189.D
 Acq On : 24 Nov 2023 20:17
 Operator : CG\JU
 Sample : 05468-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-10

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-BF110723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136189.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	16	rVB	464694	617623	7.85%	1.337%
2	5.057	500	505	516	rVB	581166	850463	10.81%	1.842%
3	5.451	566	572	575	rBV	5304392	6008575	76.35%	13.011%
4	6.445	735	741	744	rBV	4939203	6204266	78.83%	13.434%
5	6.804	799	802	806	rBV	1008414	820732	10.43%	1.777%
6	7.369	892	898	901	rBV	3548922	3853994	48.97%	8.345%
7	8.081	1015	1019	1023	rBV	1317757	1153925	14.66%	2.499%
8	9.169	1197	1204	1206	rBV	8027906	7870033	100.00%	17.041%
9	9.281	1220	1223	1233	rVB2	85672	88964	1.13%	0.193%
10	9.839	1313	1318	1321	rBV	1745086	1329342	16.89%	2.879%
11	10.633	1448	1453	1456	rBV	4740073	4700378	59.73%	10.178%
12	11.328	1568	1571	1574	rBV	1482398	1301142	16.53%	2.817%
13	11.875	1659	1664	1672	rBV2	391637	442906	5.63%	0.959%
14	12.663	1794	1798	1810	rVB	163966	189962	2.41%	0.411%
15	12.933	1839	1844	1847	rBV	7479775	6731029	85.53%	14.575%
16	13.421	1918	1927	1933	rBV	1300939	1412734	17.95%	3.059%
17	13.845	1996	1999	2006	rBV2	146627	231354	2.94%	0.501%
18	13.980	2017	2022	2025	rBV	898500	796471	10.12%	1.725%
19	15.463	2267	2274	2282	rBV	630928	766778	9.74%	1.660%
20	17.680	2637	2651	2660	rBV5	172475	470557	5.98%	1.019%
21	18.186	2729	2737	2747	rVB5	131063	340502	4.33%	0.737%

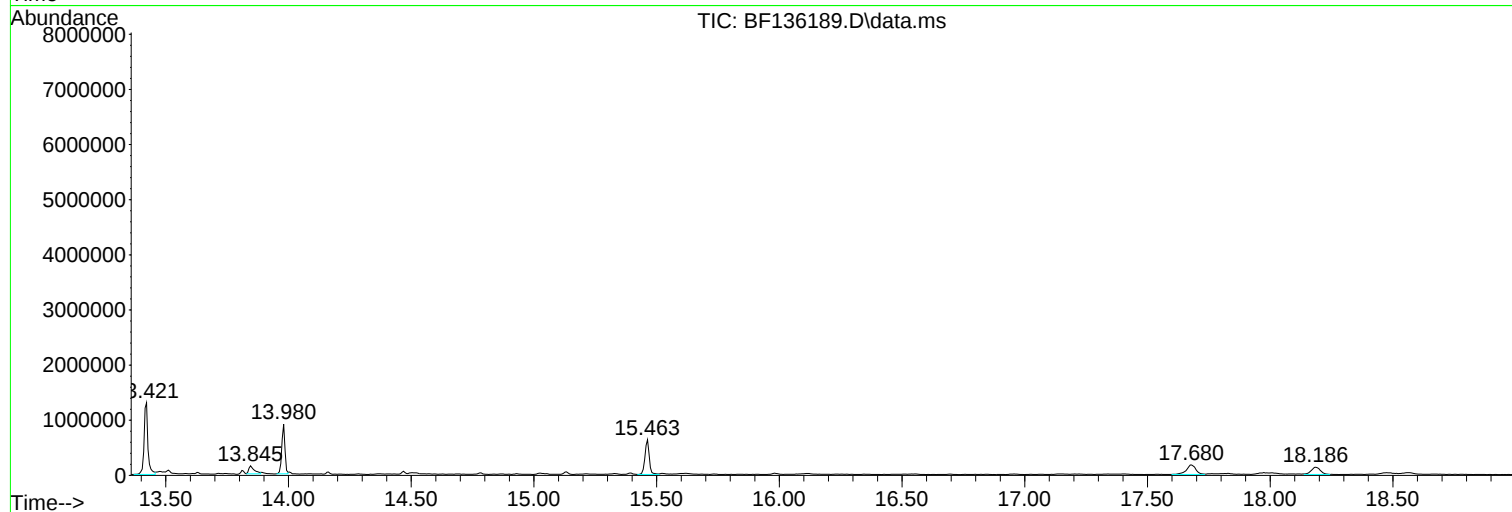
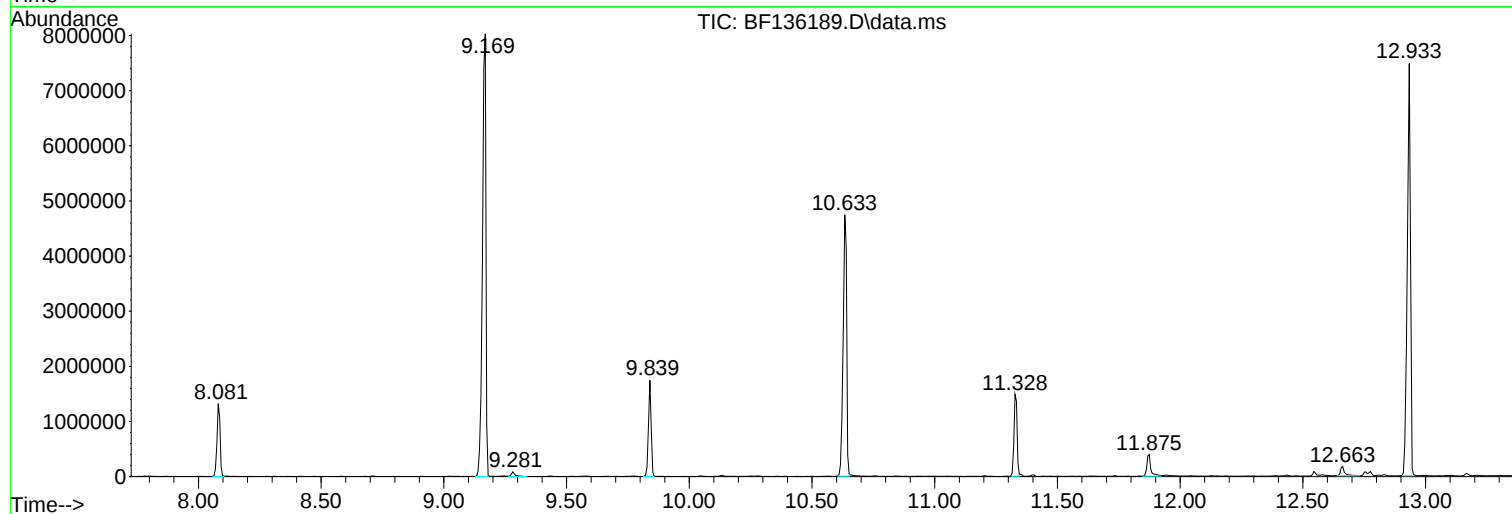
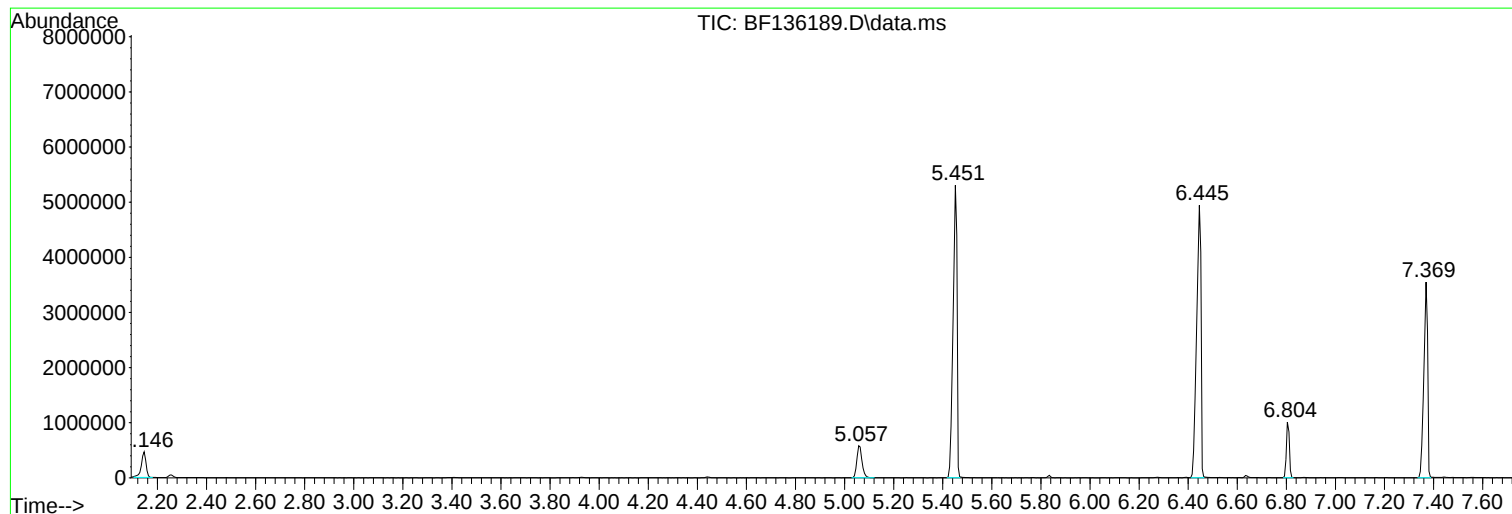
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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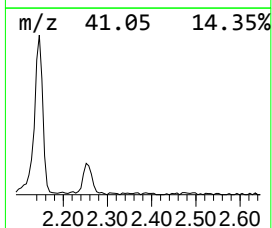
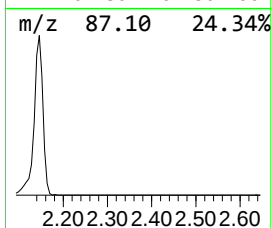
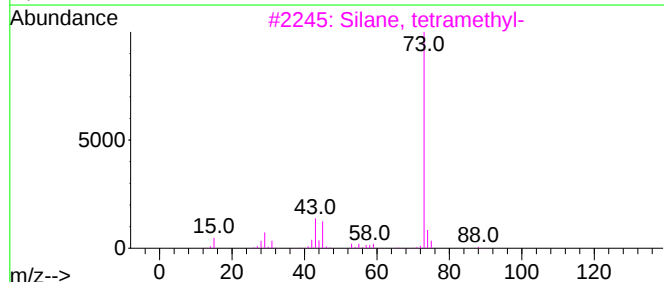
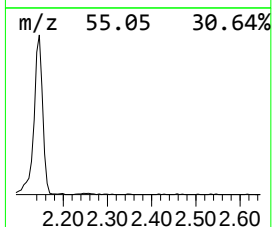
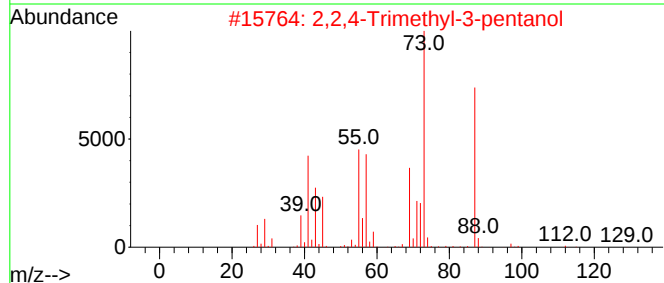
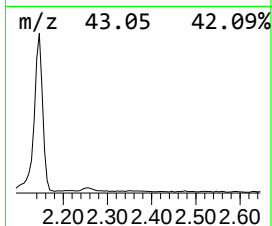
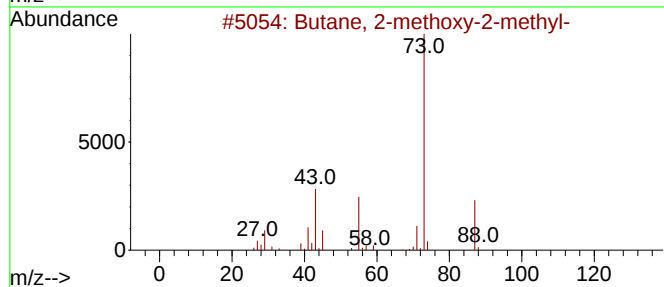
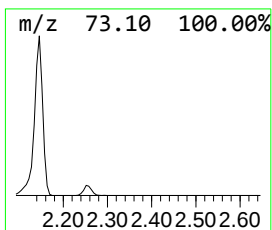
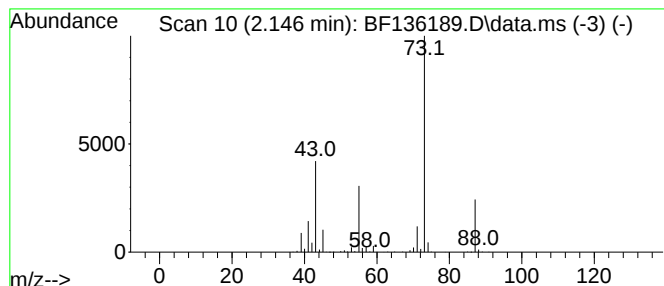
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	15.05 ng	617623	1,4-Dichlorobenzene-d4	6.804

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	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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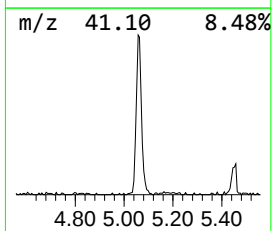
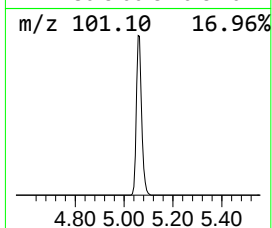
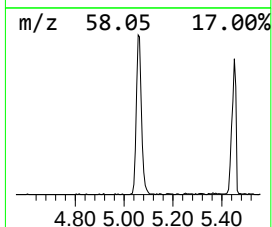
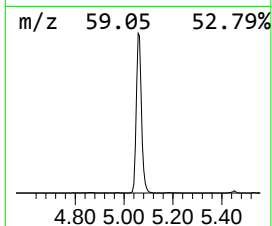
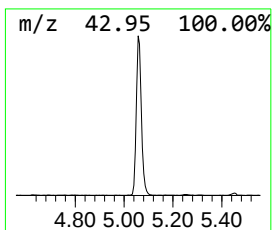
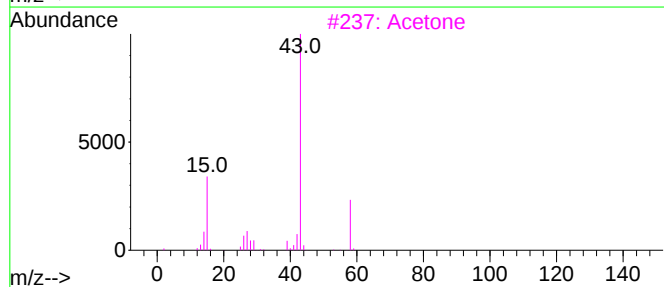
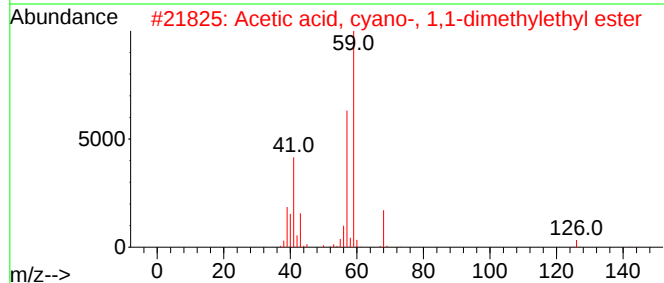
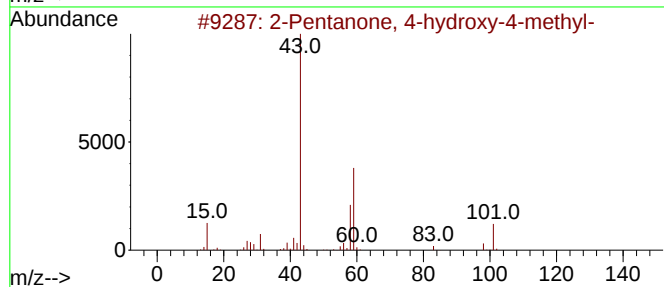
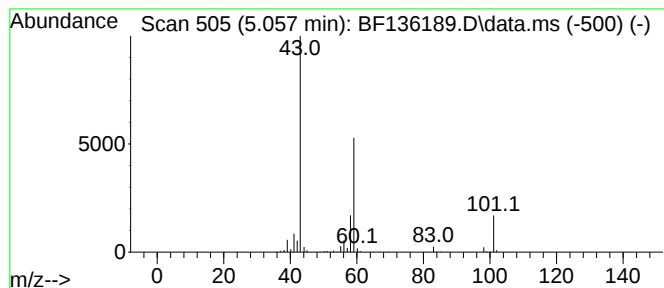
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
5.057	20.72 ng	850463	1,4-Dichlorobenzene-d4	6.804	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Acetone	58	C3H6O	000067-64-1	12
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10



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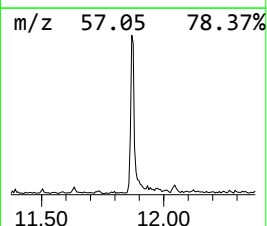
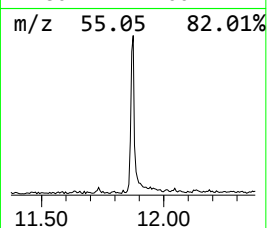
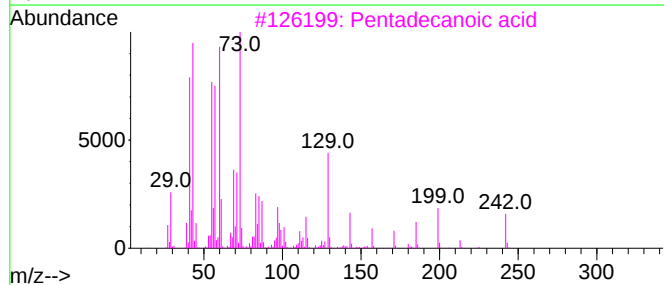
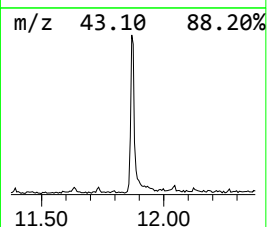
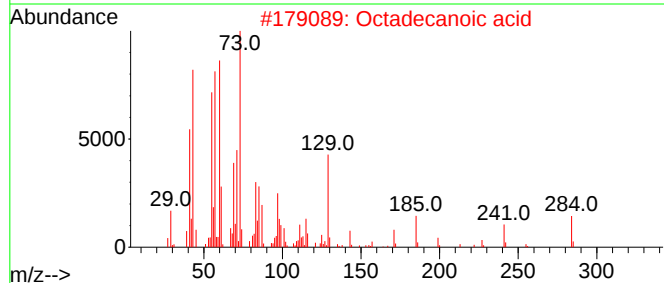
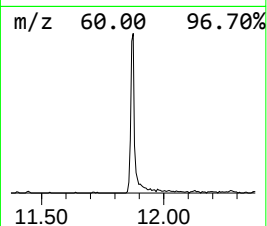
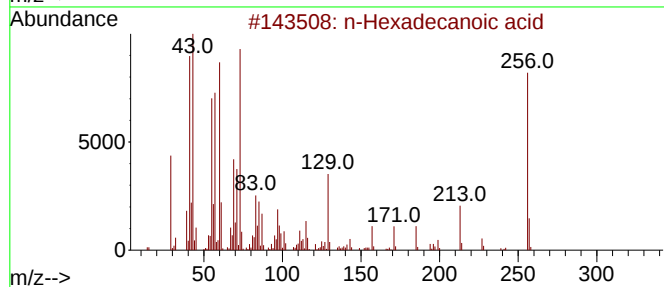
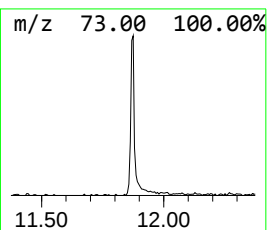
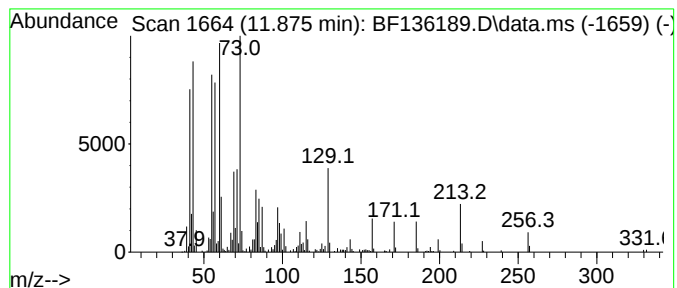
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.874	6.81 ng	442906	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Octadecanoic acid	284	C18H36O2	000057-11-4	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tridecanoic acid	214	C13H26O2	000638-53-9	91
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	87



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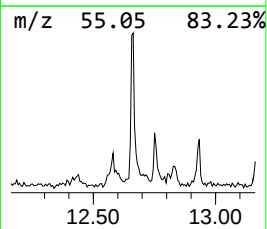
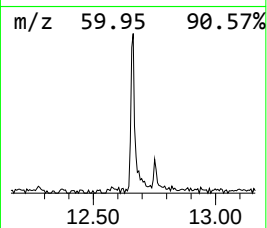
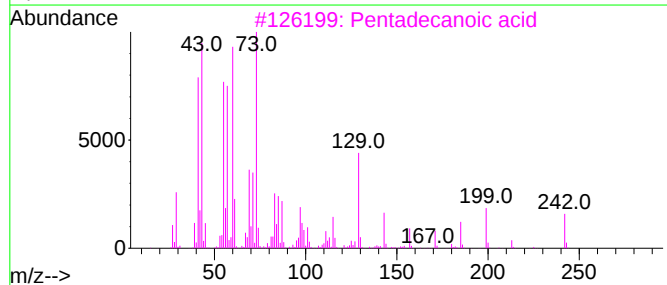
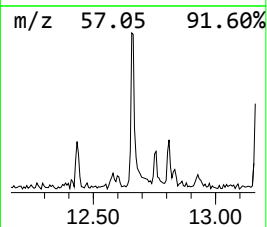
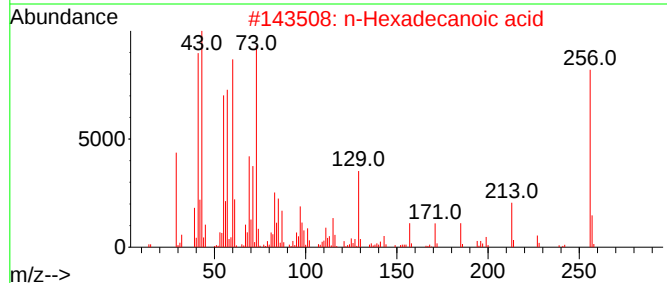
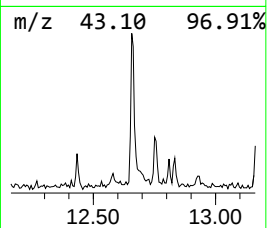
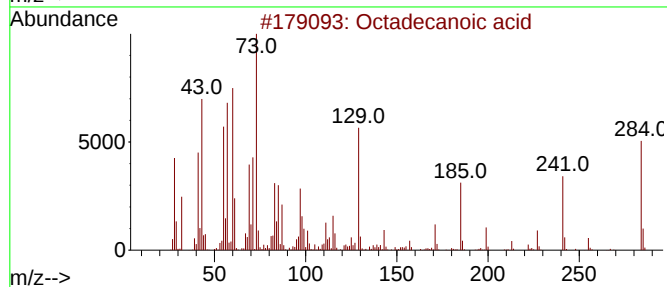
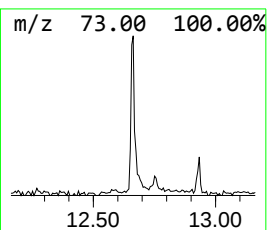
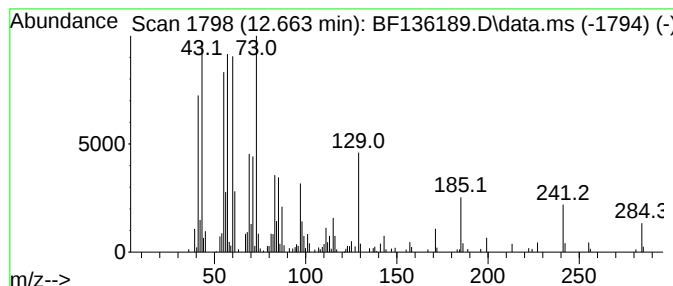
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Peak Number 4 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.663	4.77 ng	189962	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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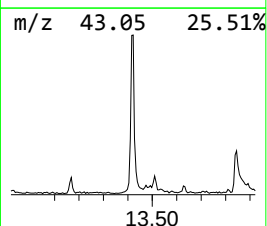
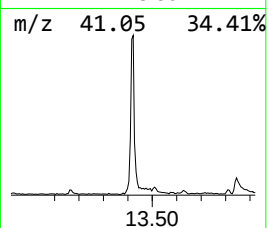
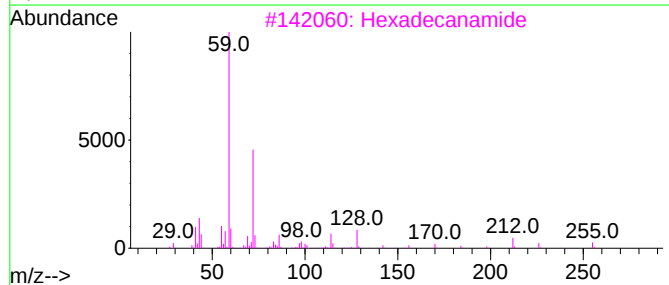
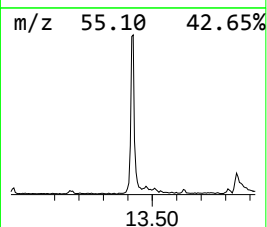
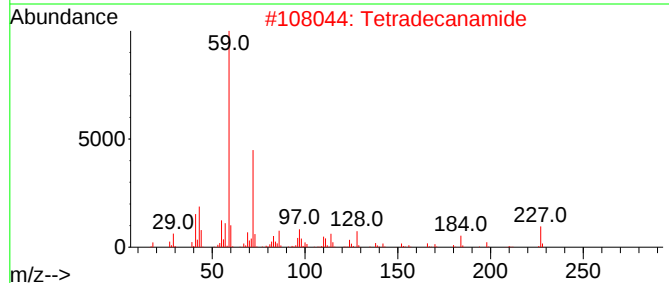
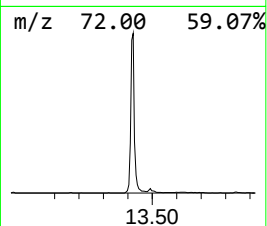
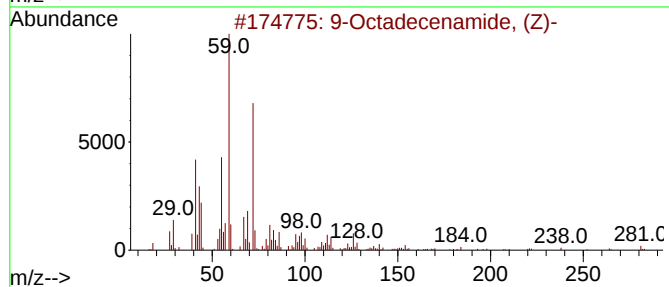
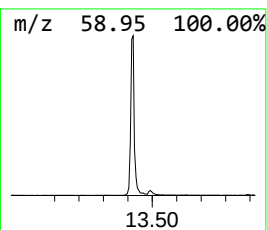
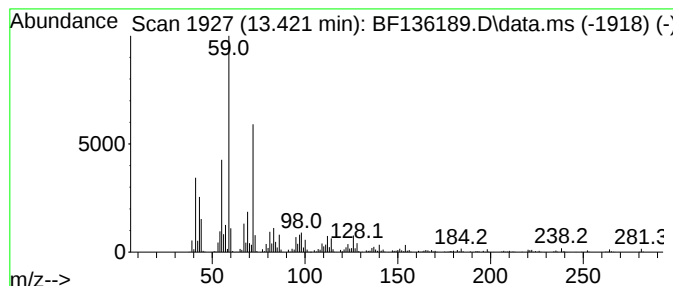
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.422	35.47 ng	1412730	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2			Tetradecanamide	227	C14H29NO	000638-58-4	93
3			Hexadecanamide	255	C16H33NO	000629-54-9	72
4			Octanamide	143	C8H17NO	000629-01-6	53
5			Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50



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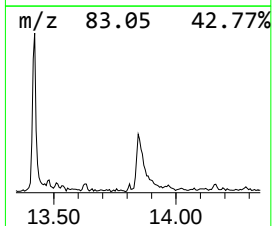
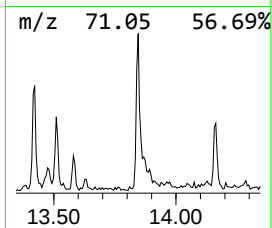
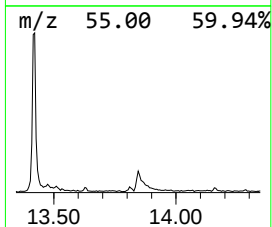
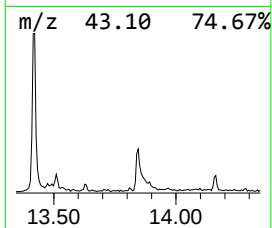
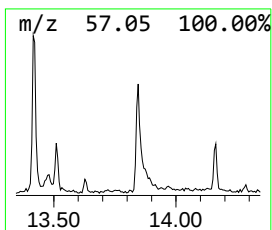
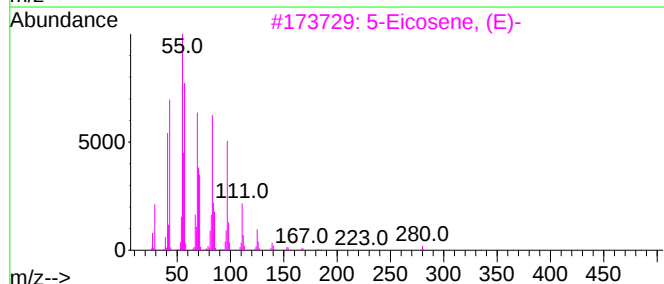
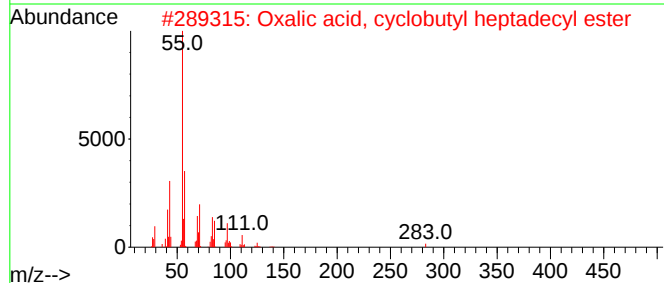
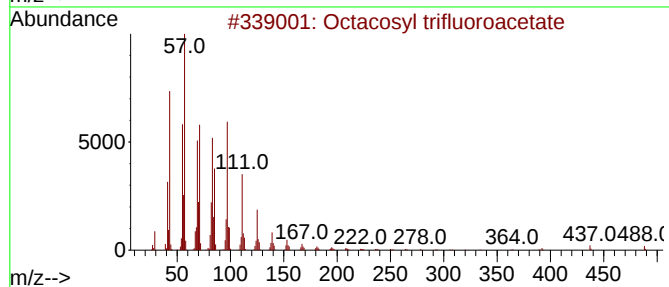
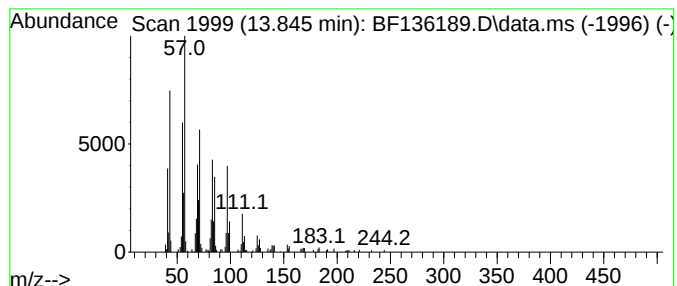
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosyl trifluoroacetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	5.81 ng	231354	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2			Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	87
3			5-Eicosene, (E)-	280	C20H40	074685-30-6	81
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	76
5			Oxalic acid, cyclobutyl hexadecy...	368	C22H40O4	1000309-70-6	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112423\
Data File : BF136189.D
Acq On : 24 Nov 2023 20:17
Operator : CG\JU
Sample : 05468-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

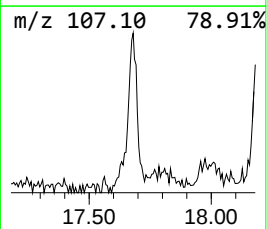
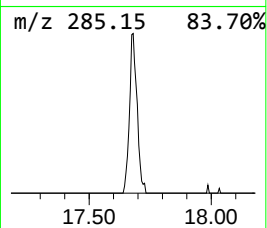
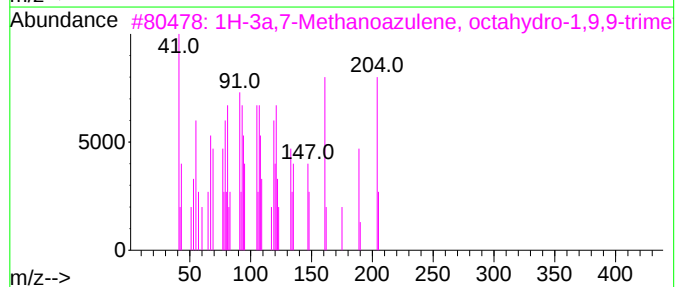
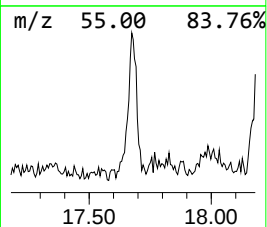
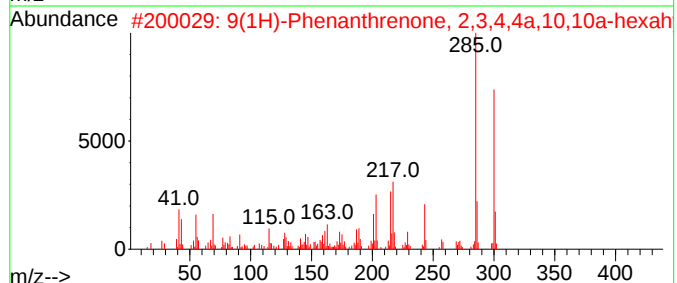
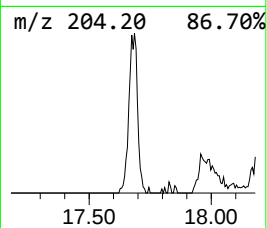
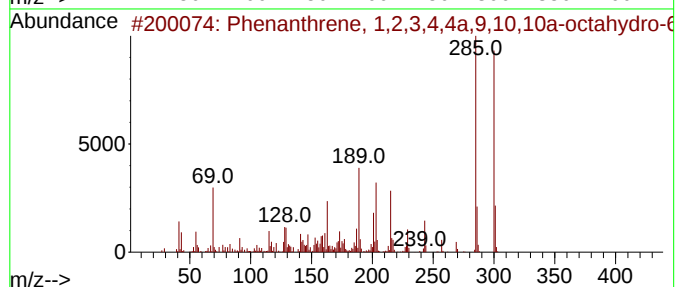
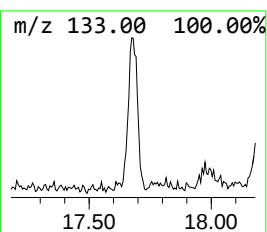
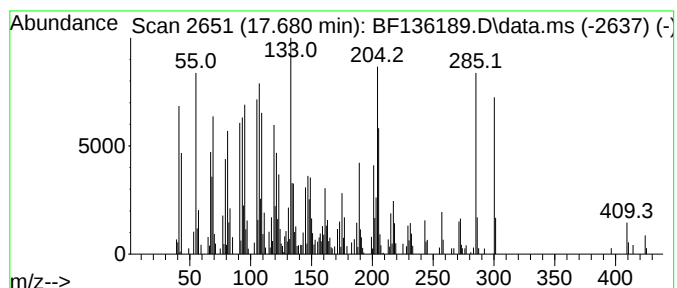
Instrument :
BNA_F
ClientSampleId :
TP-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phenanthrene, 1,2,3,4,4a,9,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.680	12.27 ng	470557	Perylene-d12	15.463	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1,2,3,4,4a,9,10,10...	300	C21H32O	010064-26-3	90
2	9(1H)-Phenanthrenone, 2,3,4,4a,1...	300	C20H28O2	000511-05-7	90
3	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	55
4	1,3-Benzodioxole, 5-(1-(4-ethoxy...	300	C18H20O4	090632-70-5	53
5	D-Friedoolean-14-en-3-one	424	C30H48O	000514-07-8	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112423\
Data File : BF136189.D
Acq On : 24 Nov 2023 20:17
Operator : CG\JU
Sample : 05468-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

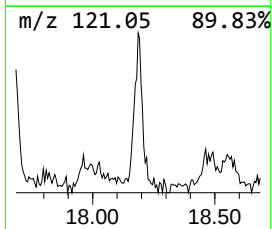
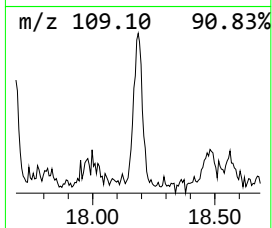
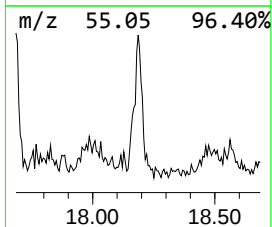
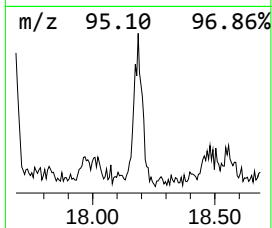
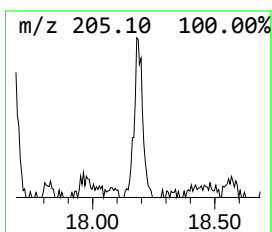
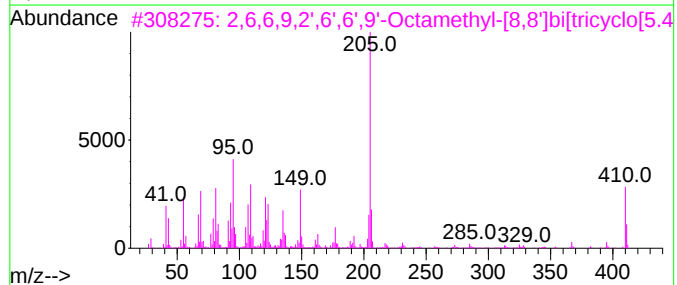
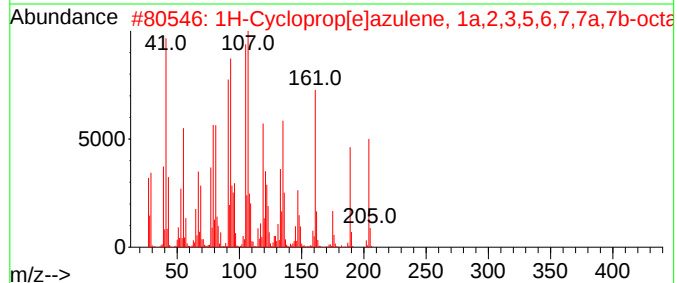
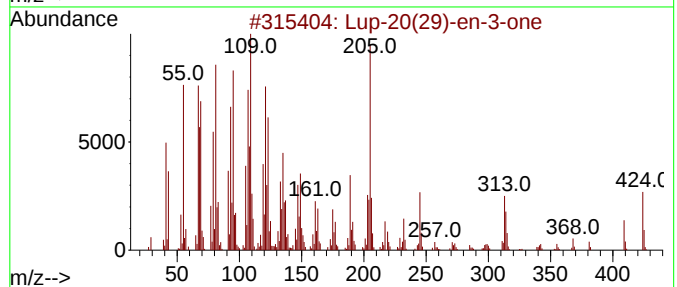
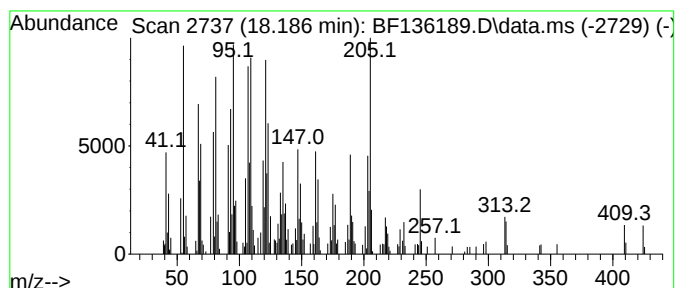
Instrument :
BNA_F
ClientSampleId :
TP-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Lup-20(29)-en-3-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.186	8.88 ng	340502	Perylene-d12	15.463	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	99
2	1H-Cycloprop[e]azulene, 1a,2,3,5...	204	C15H24	021747-46-6	53
3	2,6,6,9,2',6',6',9'-Octamethyl-[...]	410	C30H50	1000189-48-2	53
4	D:C-Friedoolean-8-en-3-one	424	C30H48O	022611-26-3	50
5	6,10-Dimethyl-3-(1-methylethylid...	206	C15H26	069239-71-0	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112423\
Data File : BF136189.D
Acq On : 24 Nov 2023 20:17
Operator : CG\JU
Sample : 05468-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110723.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	15.1	ng	617623	1	6.804	820732	20.0
2-Pentanone, 4-...	5.057	20.7	ng	850463	1	6.804	820732	20.0
n-Hexadecanoic ...	11.874	6.8	ng	442906	4	11.328	1301140	20.0
Octadecanoic acid	12.663	4.8	ng	189962	5	13.980	796471	20.0
9-Octadecenamid...	13.422	35.5	ng	1412730	5	13.980	796471	20.0
Octacosyl trifl...	13.845	5.8	ng	231354	5	13.980	796471	20.0
Phenanthrene, 1...	17.680	12.3	ng	470557	6	15.463	766778	20.0
Lup-20(29)-en-3...	18.186	8.9	ng	340502	6	15.463	766778	20.0