

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092822\
 Data File : BF130448.D
 Acq On : 28 Sep 2022 15:04
 Operator : CG\JU
 Sample : N4815-02
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SAND-FILTER-2

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-BF091422.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130448.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.828	461	466	478	rVB	153520	199838	7.27%	1.124%
2	5.251	533	538	541	rBV	2245142	2063331	75.05%	11.602%
3	6.286	709	714	730	rBV	2043857	2167666	78.85%	12.188%
4	6.645	771	775	778	rBV	763332	603292	21.94%	3.392%
5	7.210	866	871	874	rBV	1560885	1414023	51.43%	7.951%
6	7.928	981	993	996	rBV	962014	846507	30.79%	4.760%
7	9.004	1171	1176	1179	rBV	3430535	2749163	100.00%	15.458%
8	9.133	1192	1198	1206	rVB	44029	64349	2.34%	0.362%
9	9.675	1286	1290	1294	rBV	1111068	860367	31.30%	4.838%
10	10.463	1420	1424	1435	rBV	1252466	1096905	39.90%	6.168%
11	11.157	1538	1542	1545	rBV	944176	766439	27.88%	4.309%
12	11.557	1606	1610	1614	rVB	32549	34645	1.26%	0.195%
13	11.698	1625	1634	1652	rBV	304540	509888	18.55%	2.867%
14	11.957	1675	1678	1682	rVB2	36340	47907	1.74%	0.269%
15	12.263	1727	1730	1736	rVB4	67948	78329	2.85%	0.440%
16	12.345	1740	1744	1749	rBV2	38058	56785	2.07%	0.319%
17	12.480	1761	1767	1778	rBV	401766	600789	21.85%	3.378%
18	12.745	1807	1812	1815	rVB	2244135	2066881	75.18%	11.621%
19	13.786	1985	1989	1996	rVB	583926	505411	18.38%	2.842%
20	13.886	1998	2006	2015	rBV4	73168	180875	6.58%	1.017%
21	14.868	2170	2173	2178	rVB	44365	42637	1.55%	0.240%
22	15.174	2220	2225	2229	rBV	497669	540742	19.67%	3.040%
23	15.604	2294	2298	2306	rVB	52795	77322	2.81%	0.435%
24	16.056	2371	2375	2386	rBV7	25011	81202	2.95%	0.457%
25	18.333	2755	2762	2771	rVB9	49590	129706	4.72%	0.729%

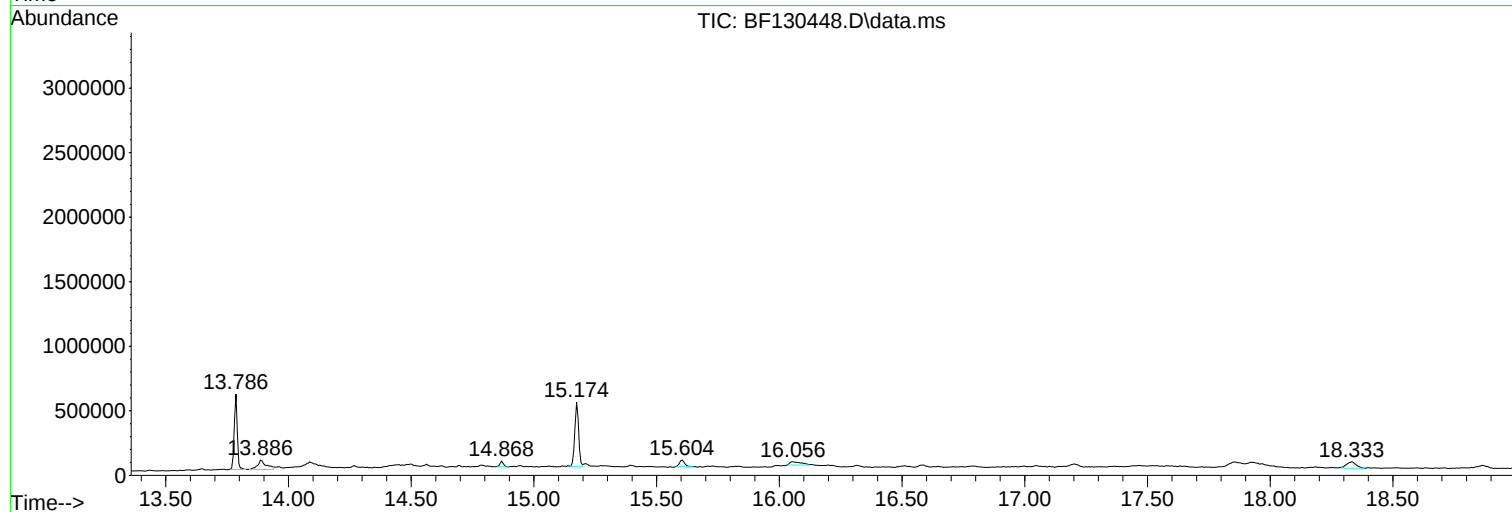
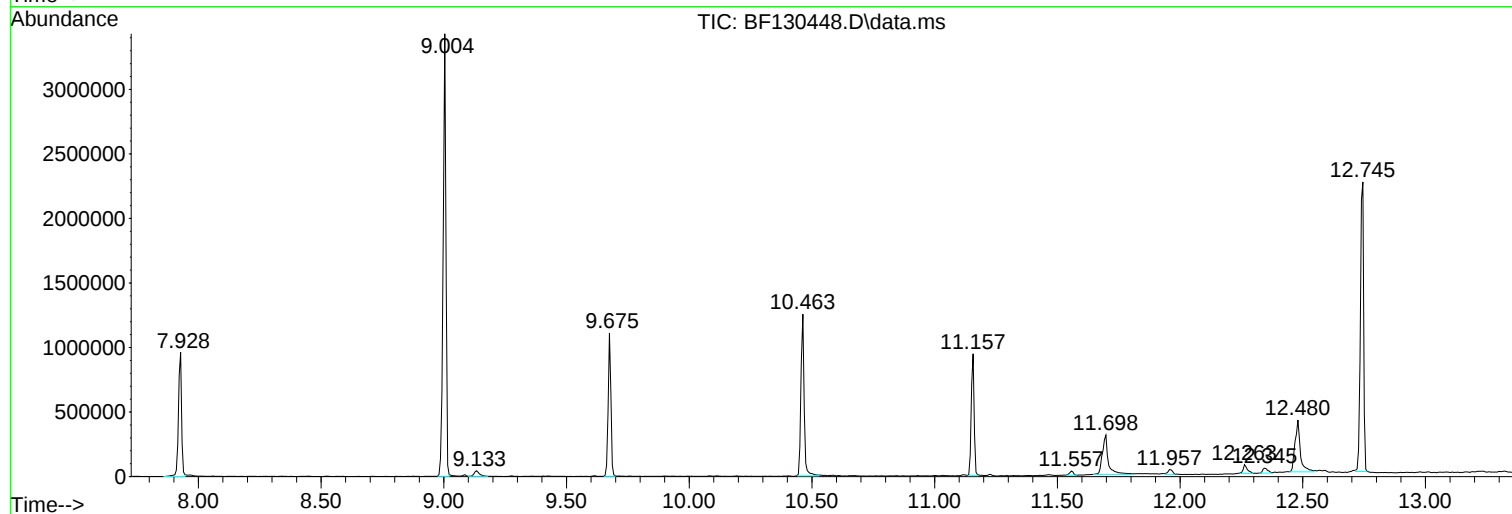
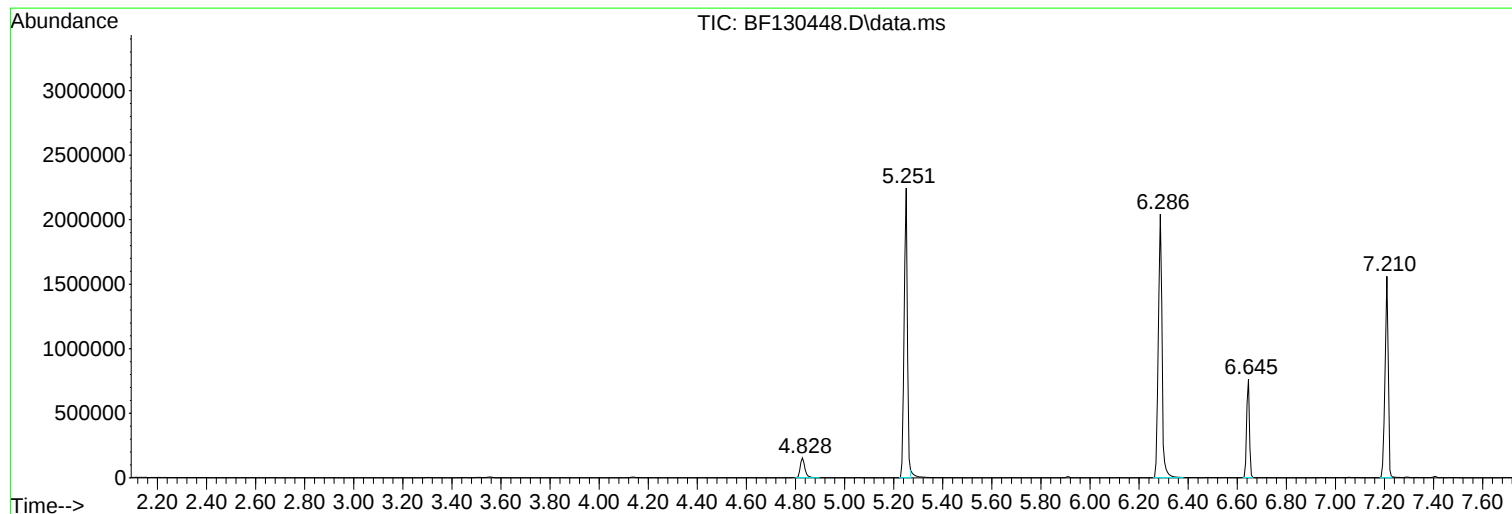
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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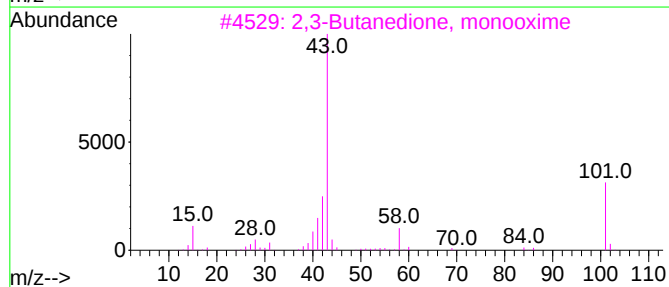
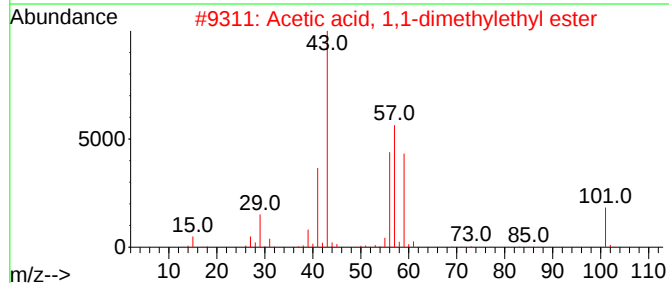
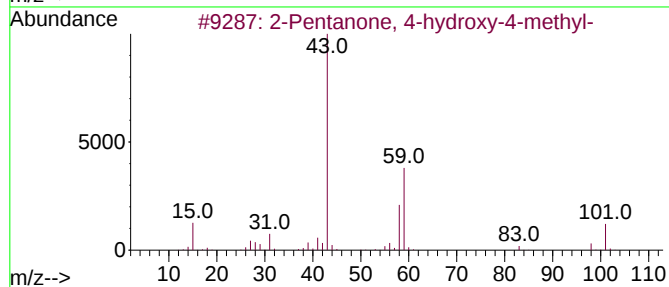
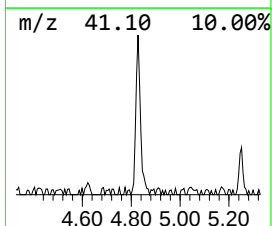
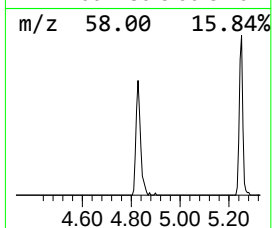
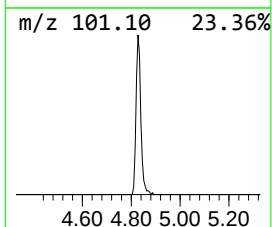
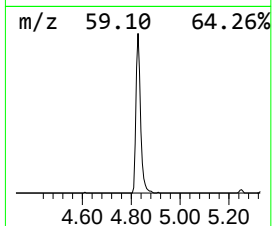
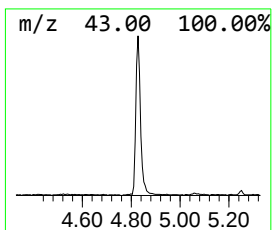
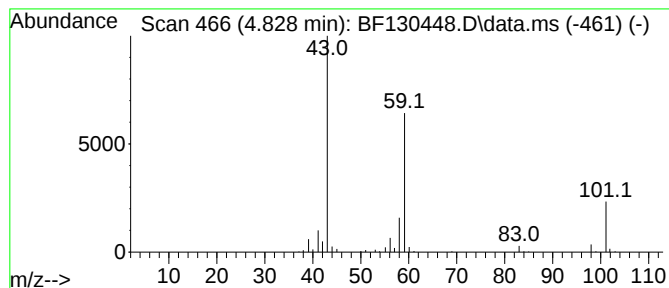
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.828	6.62 ng	199838	1,4-Dichlorobenzene-d4	6.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
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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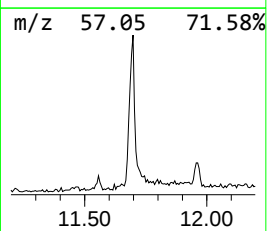
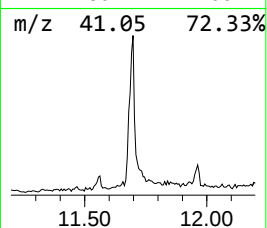
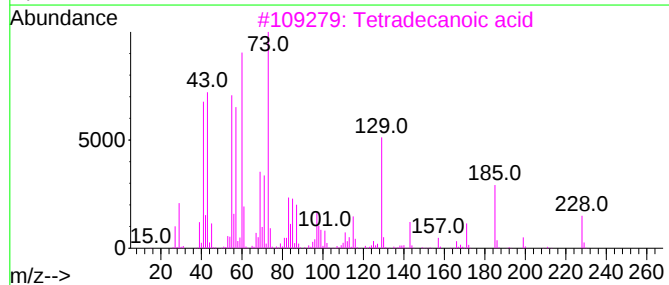
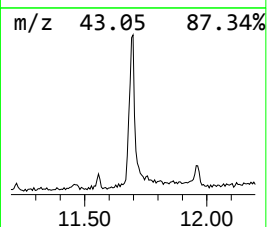
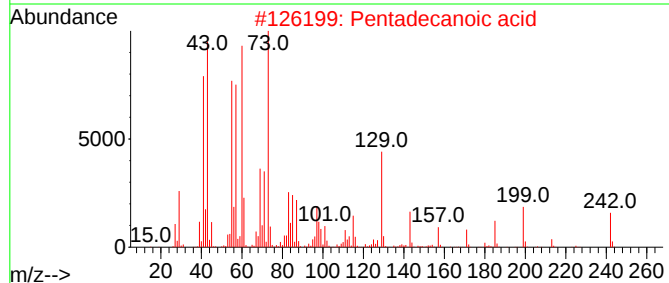
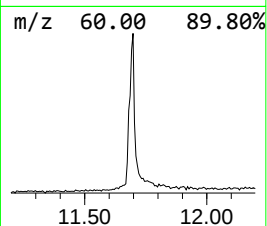
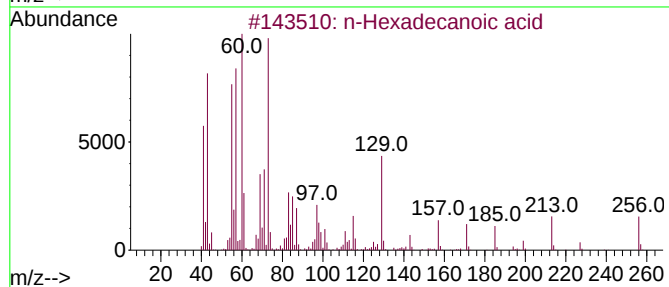
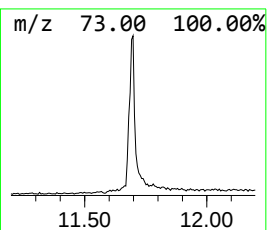
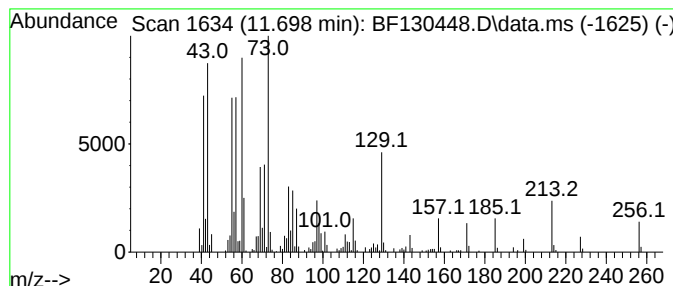
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.698	13.31 ng	509888	Phenanthrene-d10	11.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4			n-Decanoic acid	172	C10H20O2	000334-48-5	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	83



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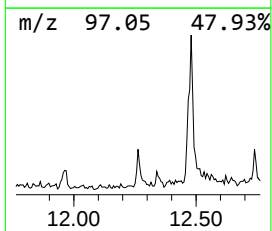
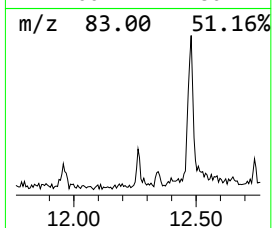
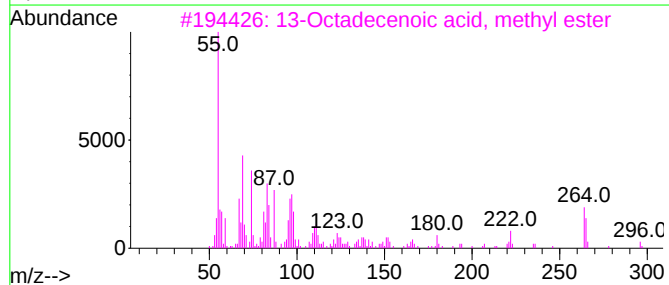
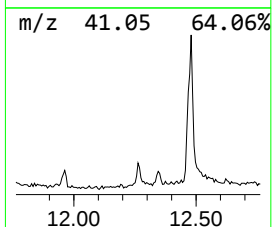
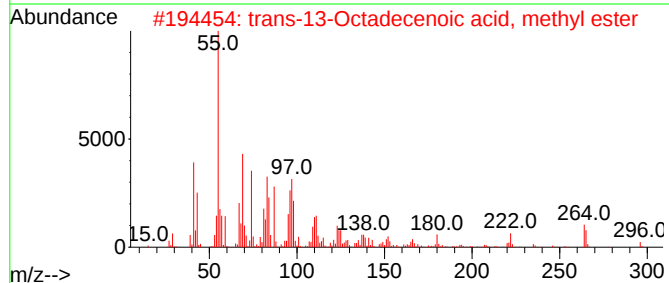
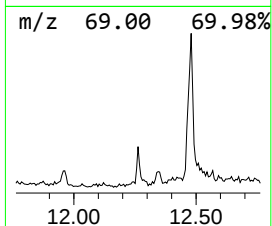
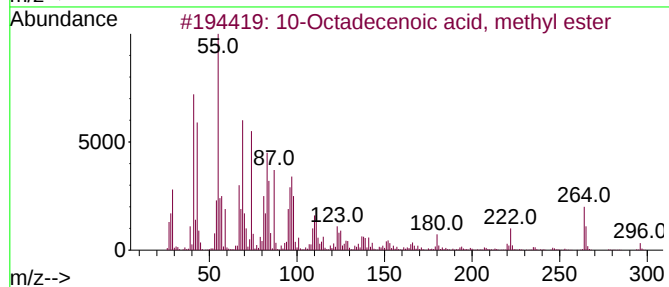
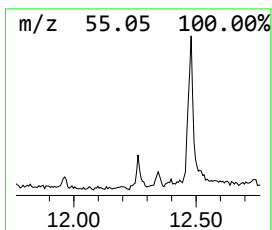
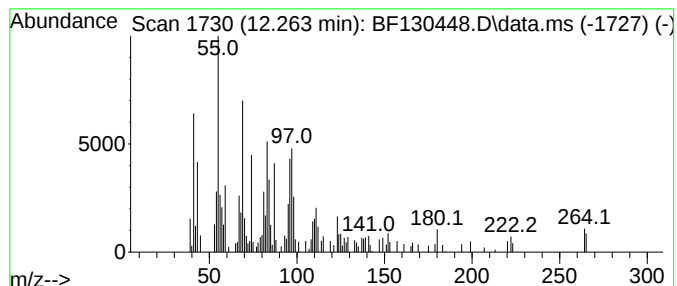
Instrument :
BNA_F
ClientSampleId :
SAND-FILTER-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 10-Octadecenoic acid, methy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.263	2.04 ng	78329	Phenanthrene-d10	11.157	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	83
2	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	74
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	72
4	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	68
5	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	64



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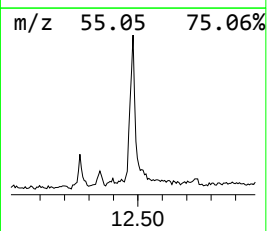
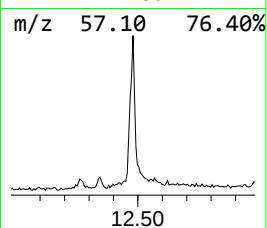
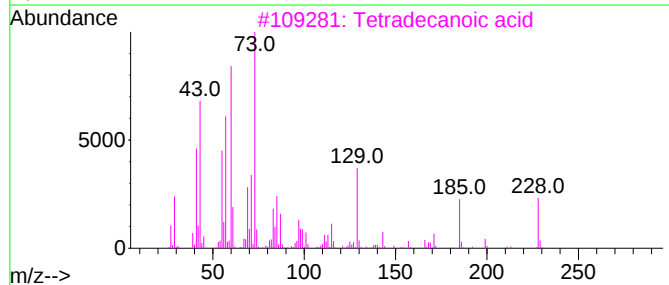
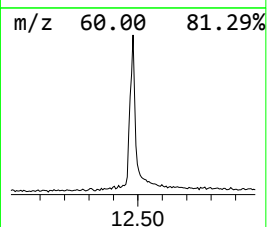
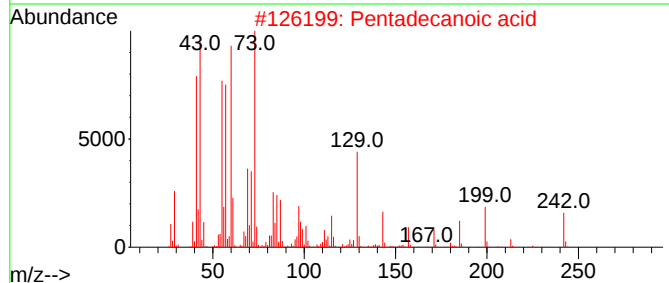
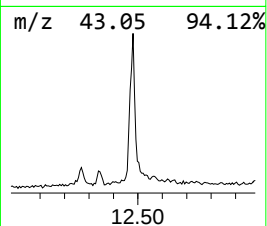
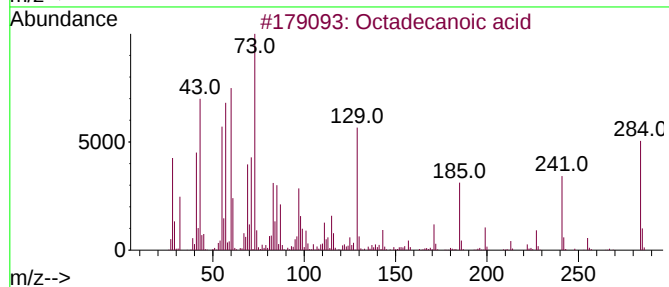
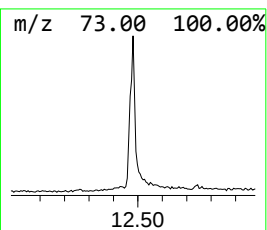
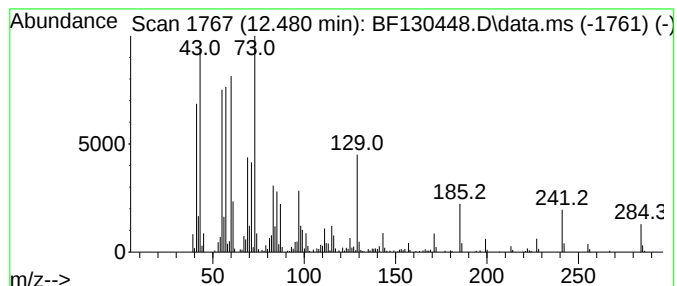
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Peak Number 4 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.480	23.77 ng	600789	Chrysene-d12	13.786

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	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	74
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72



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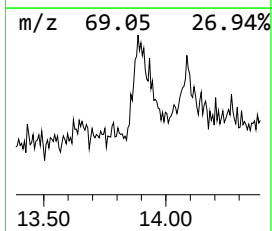
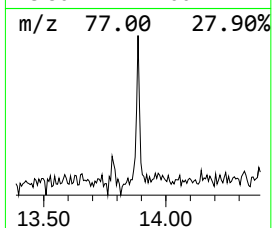
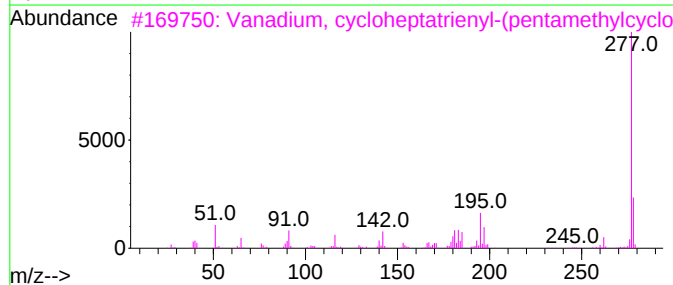
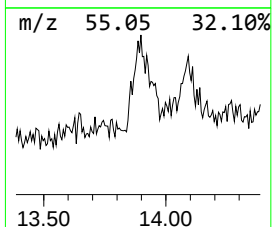
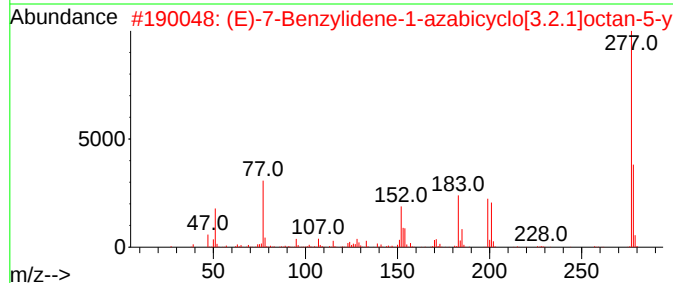
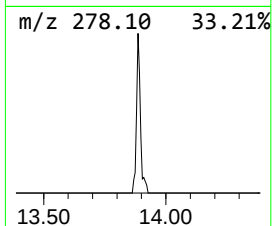
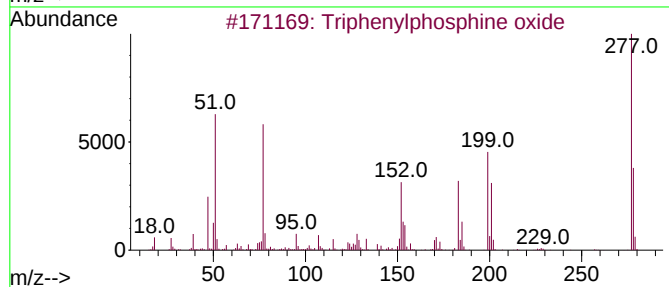
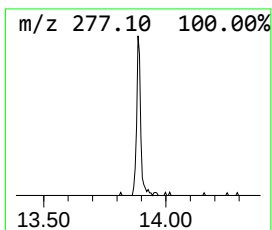
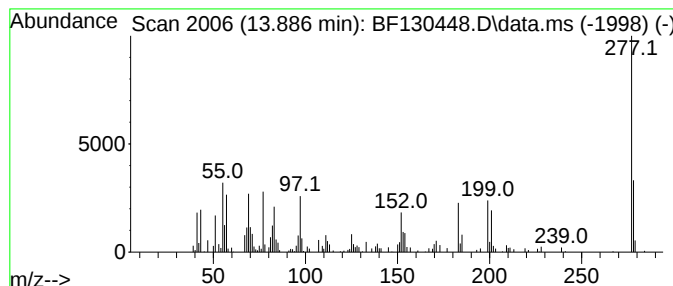
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	7.16 ng	180875	Chrysene-d12	13.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	90
3			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43
4			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	40
5			Acetamide, N-(2,5-dimethoxypheny...	277	C14H15N03S	1000306-90-6	37



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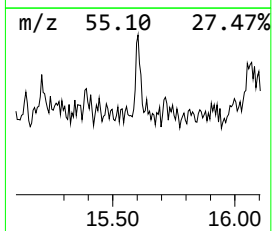
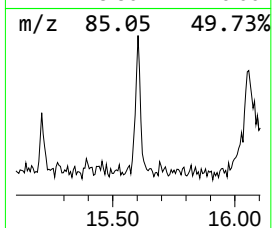
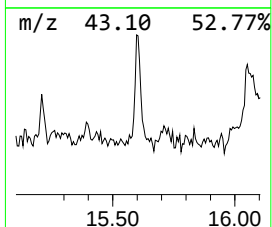
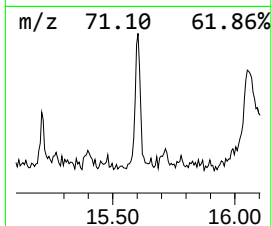
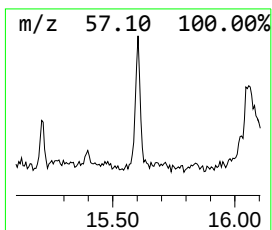
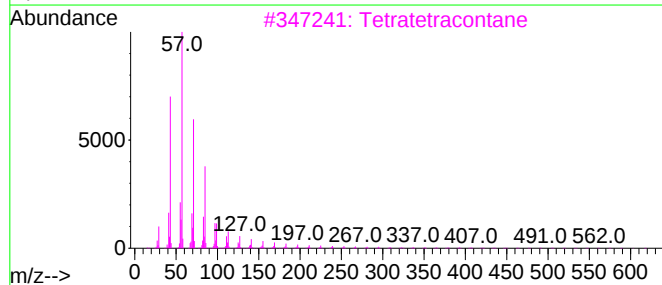
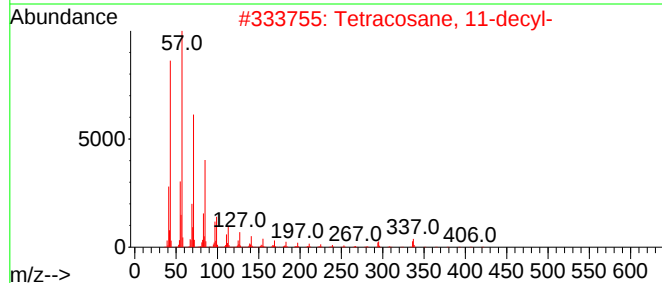
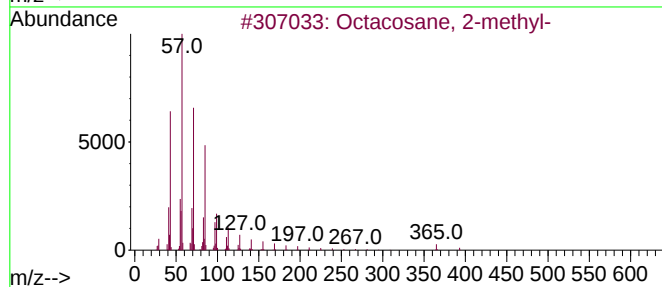
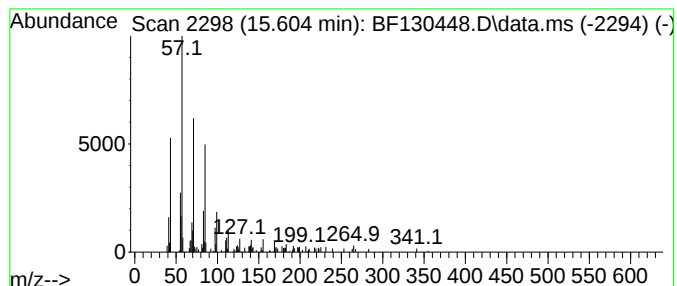
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.604	2.86 ng	77322	Perylene-d12	15.174

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	91
3			Tetratetracontane	619	C44H90	007098-22-8	91
4			Docosane, 11-decyl-	451	C32H66	055401-55-3	91
5			2-Methylhexacosane	380	C27H56	001561-02-0	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092822\
Data File : BF130448.D
Acq On : 28 Sep 2022 15:04
Operator : CG\JU
Sample : N4815-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAND-FILTER-2

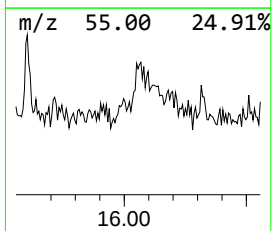
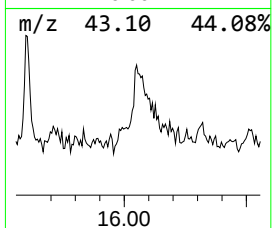
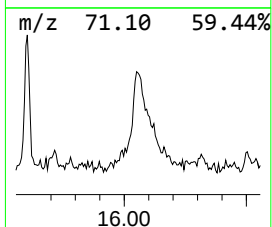
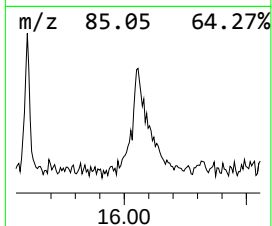
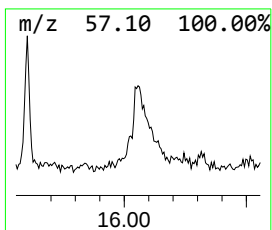
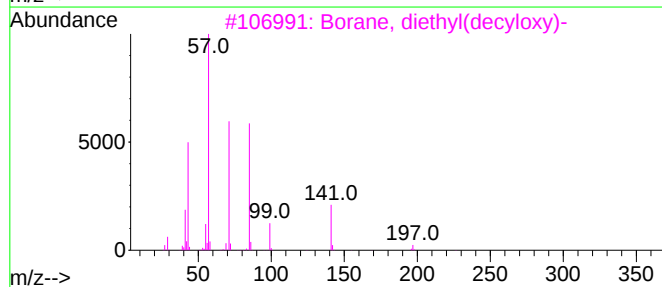
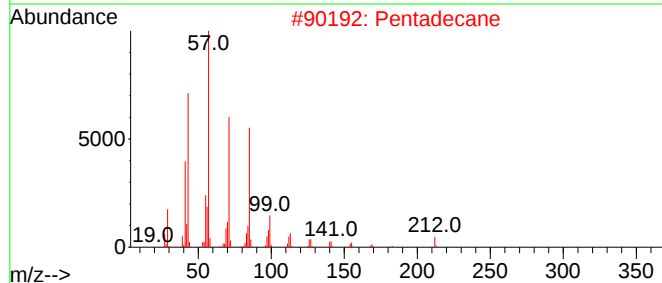
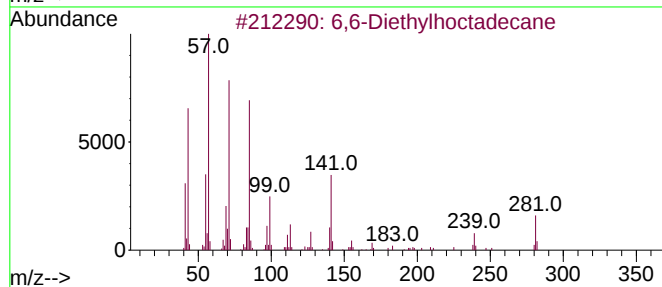
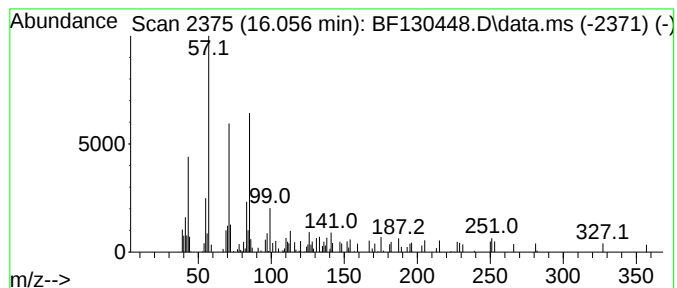
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 6,6-Diethylhooctadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.057	3.00 ng	81202	Perylene-d12	15.174

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6,6-Diethylhooctadecane	310	C22H46	1000360-41-8	53
2			Pentadecane	212	C15H32	000629-62-9	53
3			Borane, diethyl(decyloxy)-	226	C14H31BO	1000152-34-3	50
4			Tetradecane	198	C14H30	000629-59-4	47
5			Sulfurous acid, isohexyl pentyl ...	236	C11H24O3S	1000309-14-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092822\
Data File : BF130448.D
Acq On : 28 Sep 2022 15:04
Operator : CG\JU
Sample : N4815-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAND-FILTER-2

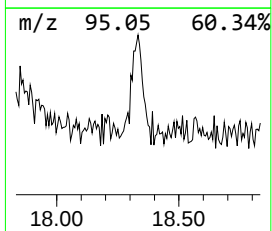
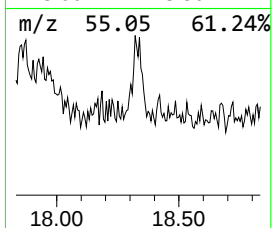
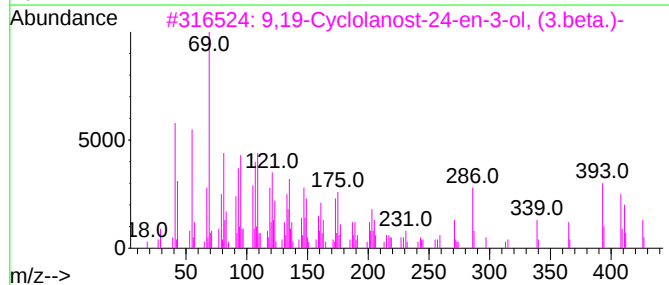
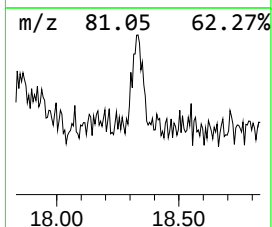
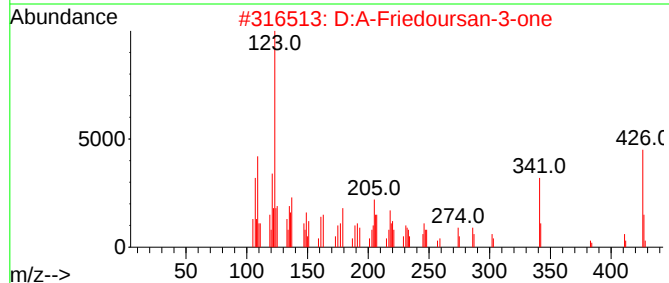
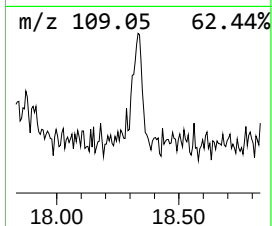
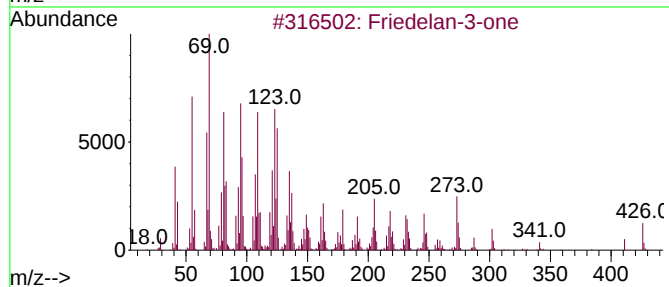
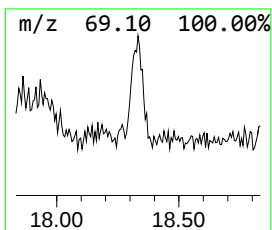
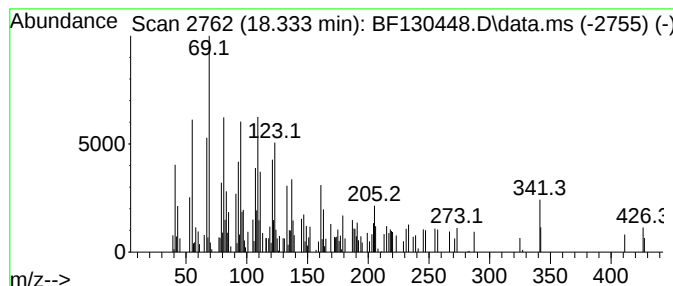
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Friedelan-3-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.333	4.80 ng	129706	Perylene-d12	15.174

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Friedelan-3-one	426	C30H50O	000559-74-0	90
2			D:A-Friedoursan-3-one	426	C30H50O	089950-00-5	47
3			9,19-Cyclolanost-24-en-3-ol, (3...	426	C30H50O	000469-38-5	45
4			Lupeol	426	C30H50O	000545-47-1	38
5			1-Formyl-2,2-dimethyl-3-cis-(2-m...	220	C15H24O	1000144-10-0	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092822\
Data File : BF130448.D
Acq On : 28 Sep 2022 15:04
Operator : CG\JU
Sample : N4815-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAND-FILTER-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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
2-Pentanone, 4-...	4.828	6.6	ng	199838	1	6.645	603292	20.0
n-Hexadecanoic ...	11.698	13.3	ng	509888	4	11.157	766439	20.0
10-Octadecenoic...	12.263	2.0	ng	78329	4	11.157	766439	20.0
Octadecanoic acid	12.480	23.8	ng	600789	5	13.786	505411	20.0
Triphenylphosph...	13.886	7.2	ng	180875	5	13.786	505411	20.0
Octacosane, 2-m...	15.604	2.9	ng	77322	6	15.174	540742	20.0
6,6-Diethylhocht...	16.057	3.0	ng	81202	6	15.174	540742	20.0
Friedelan-3-one	18.333	4.8	ng	129706	6	15.174	540742	20.0