

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112823\
 Data File : BF136254.D
 Acq On : 28 Nov 2023 17:53
 Operator : CG\JU
 Sample : 05468-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-9

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-BF112723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136254.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	21	rVB	389124	524928	9.52%	1.643%
2	2.234	21	25	30	rVB3	38432	56980	1.03%	0.178%
3	5.051	498	504	515	rVB	500339	668593	12.13%	2.093%
4	5.446	565	571	574	rBV	4096700	3939785	71.45%	12.335%
5	6.440	734	740	743	rBV	3749467	3930364	71.28%	12.305%
6	6.804	798	802	805	rBV	961687	772633	14.01%	2.419%
7	7.363	891	897	900	rBV	2694985	2557245	46.38%	8.006%
8	8.081	1014	1019	1022	rBV	1219234	1055611	19.15%	3.305%
9	9.163	1197	1203	1206	rBV	5716874	5513745	100.00%	17.262%
10	9.275	1218	1222	1227	rVB	65844	61673	1.12%	0.193%
11	9.833	1313	1317	1321	rBV	1400937	1214137	22.02%	3.801%
12	10.628	1447	1452	1455	rBV	3376345	2992616	54.28%	9.369%
13	11.327	1567	1571	1574	rBV	1513874	1200800	21.78%	3.759%
14	11.869	1655	1663	1678	rBV2	306981	402079	7.29%	1.259%
15	12.657	1790	1797	1807	rBV	193702	234647	4.26%	0.735%
16	12.927	1838	1843	1846	rBV	5298335	5005347	90.78%	15.671%
17	13.845	1996	1999	2012	rBV3	79295	190678	3.46%	0.597%
18	13.980	2018	2022	2028	rVB	719062	649590	11.78%	2.034%
19	14.163	2046	2053	2062	rBV	74115	80376	1.46%	0.252%
20	15.457	2268	2273	2280	rBV2	489417	632127	11.46%	1.979%
21	15.974	2355	2361	2374	rBV2	34764	80375	1.46%	0.252%
22	17.139	2552	2559	2565	rBV5	23277	57823	1.05%	0.181%
23	18.180	2726	2736	2745	rVB10	44596	118851	2.16%	0.372%

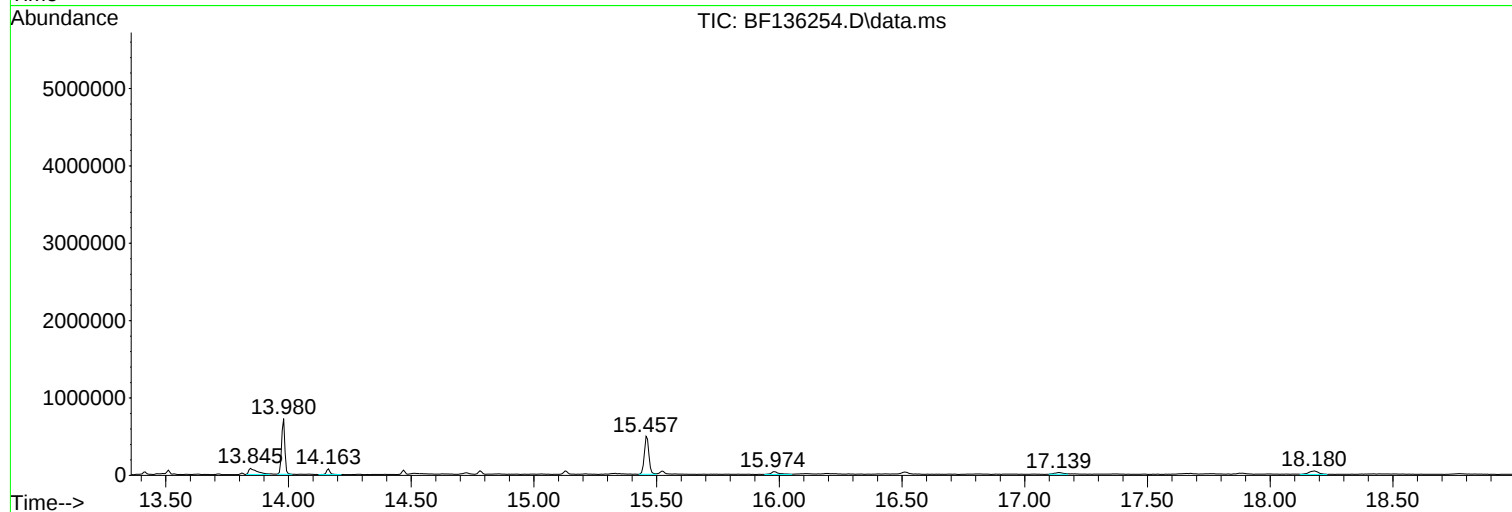
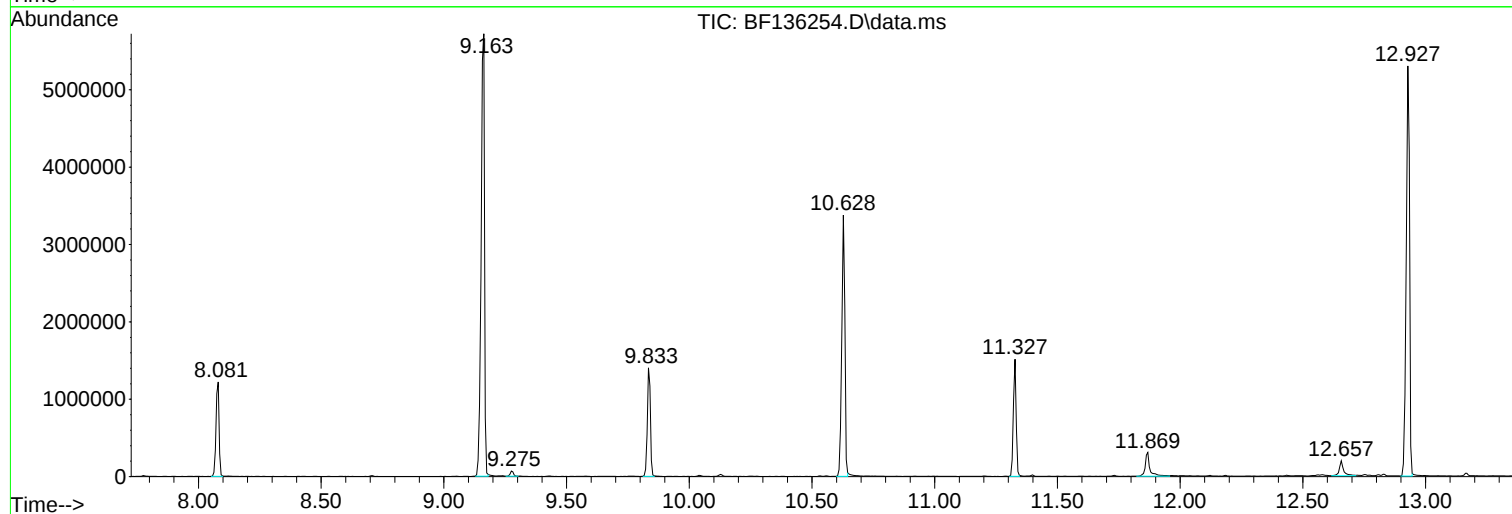
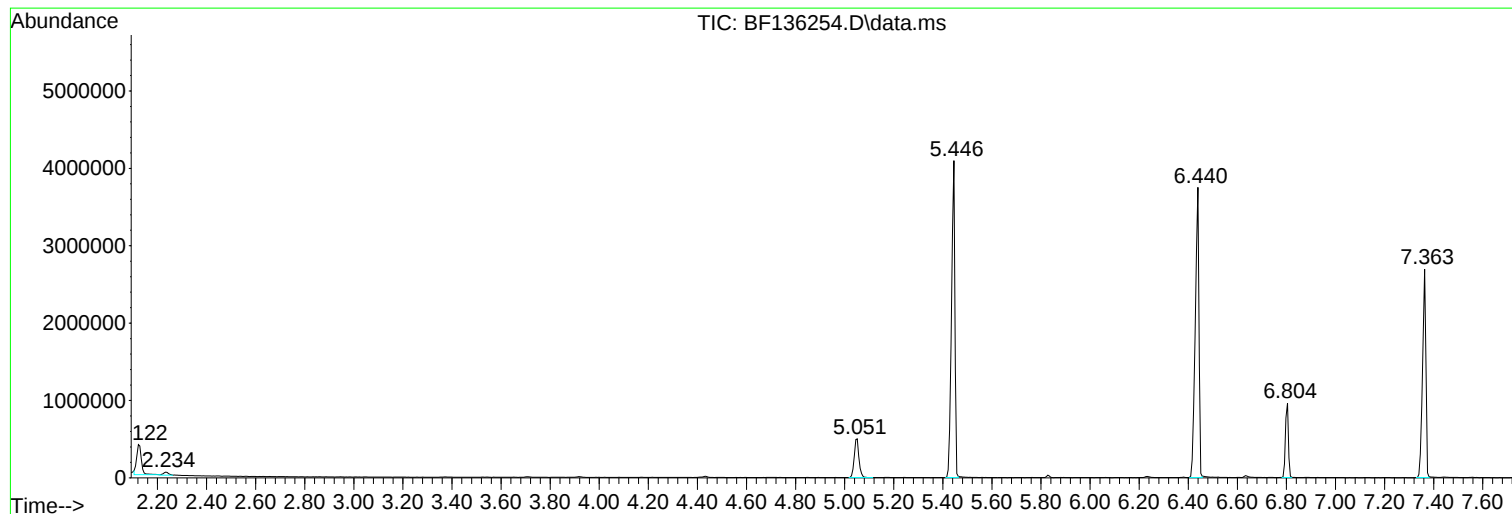
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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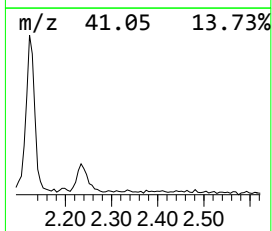
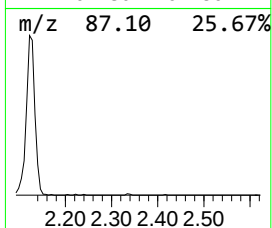
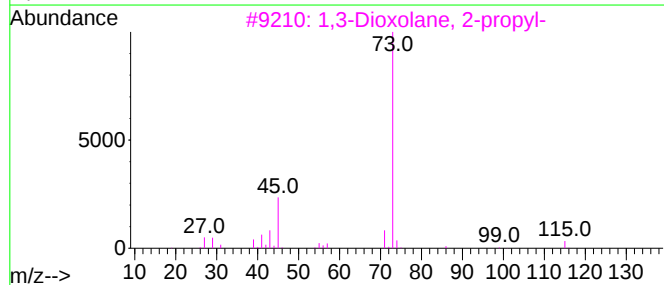
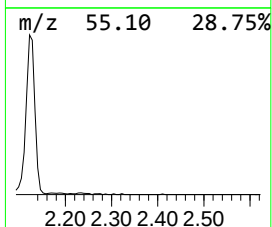
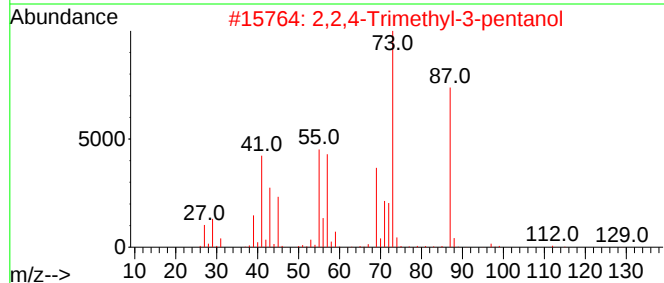
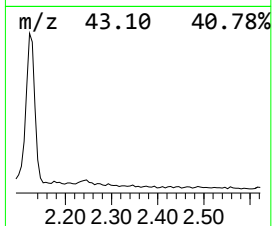
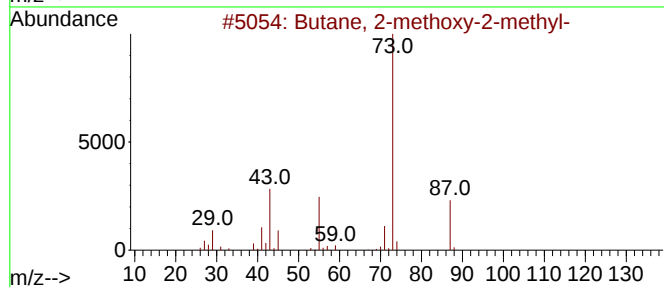
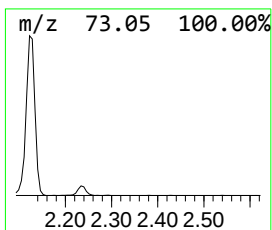
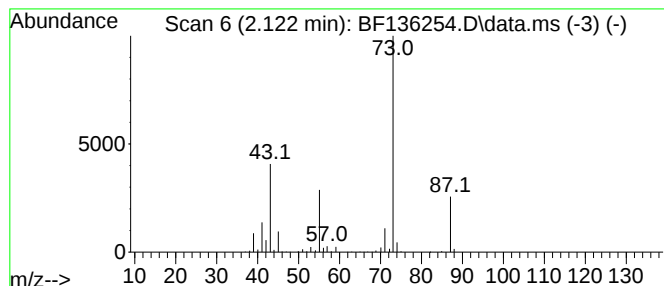
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	13.59 ng	524928	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	40
3			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22



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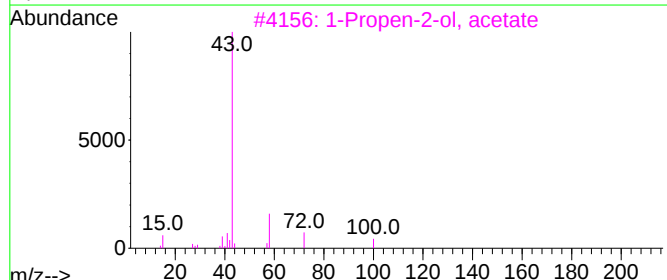
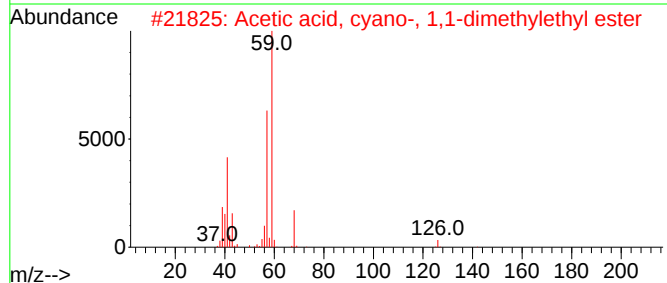
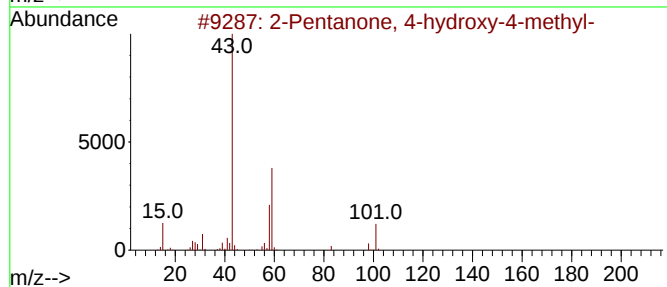
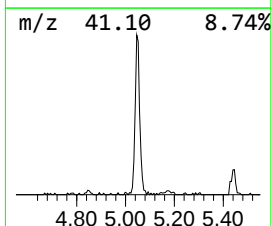
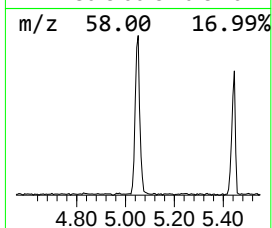
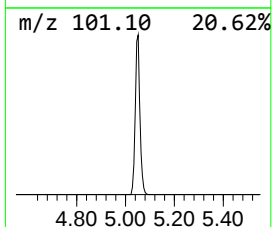
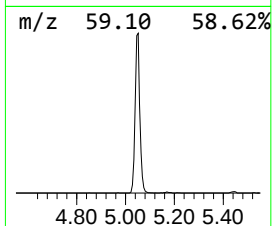
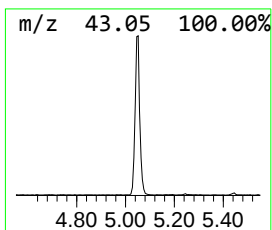
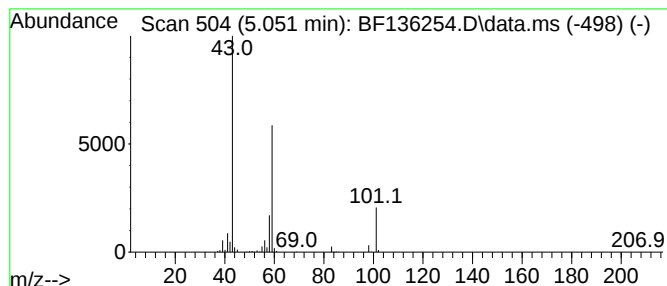
Instrument :
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ClientSampleId :
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.051	17.31 ng	668593	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	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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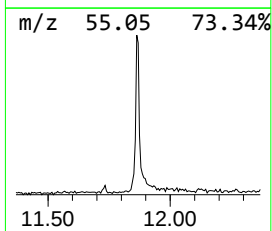
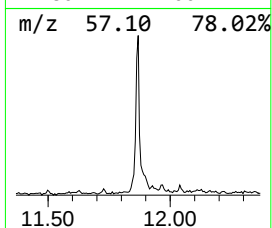
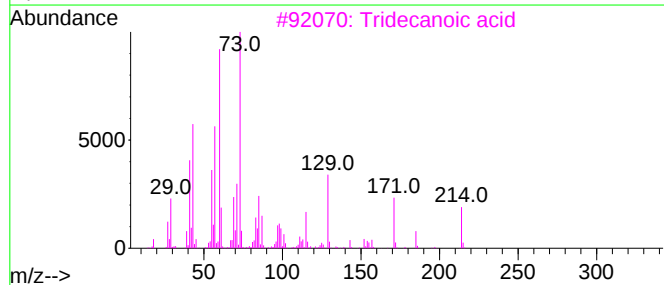
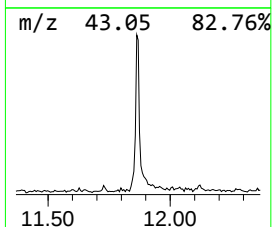
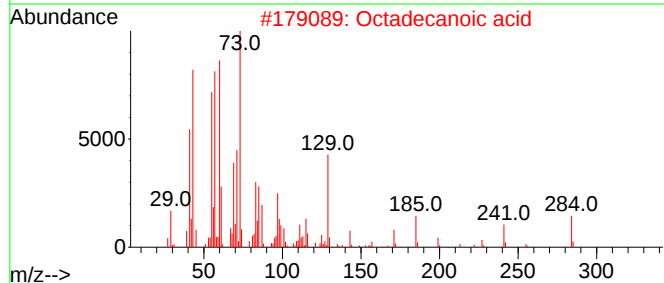
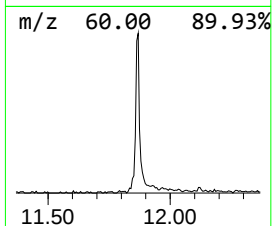
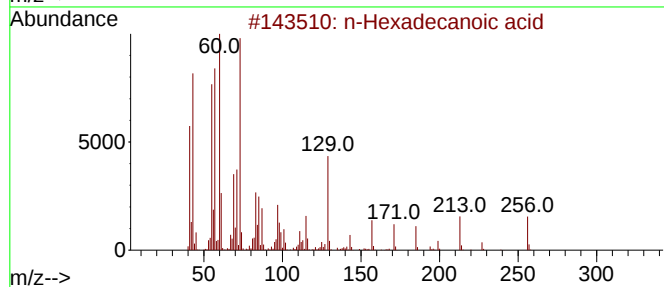
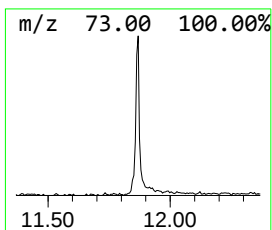
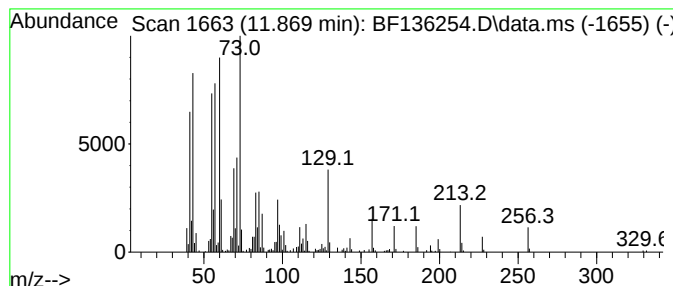
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.869	6.70 ng	402079	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	80
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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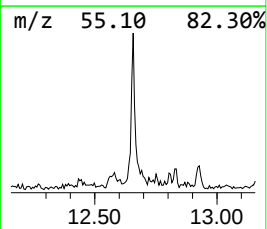
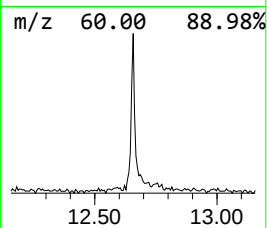
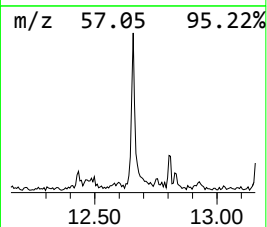
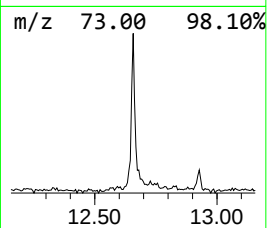
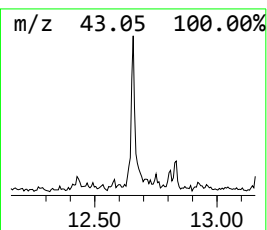
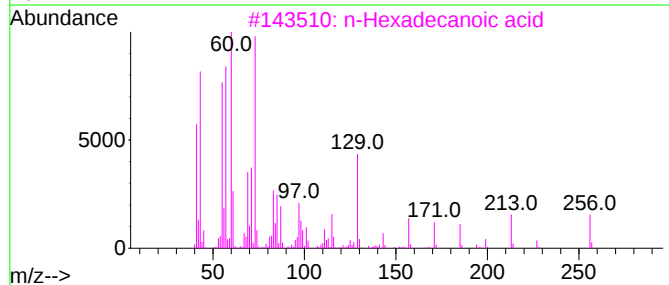
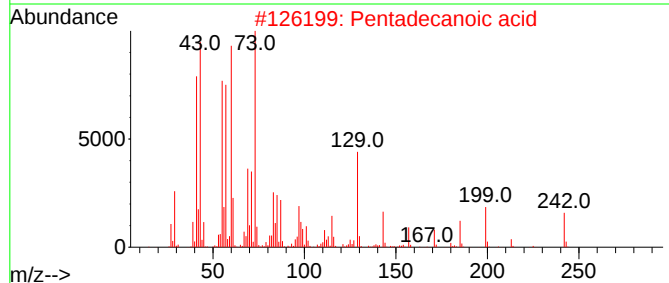
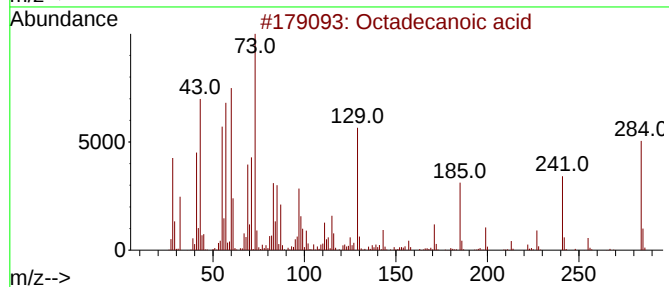
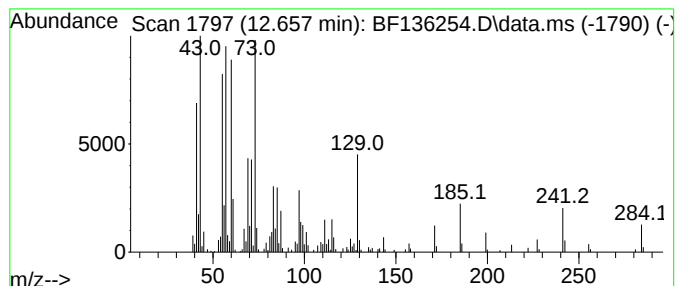
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.657	7.22 ng	234647	Chrysene-d12	13.980

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	94
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	74



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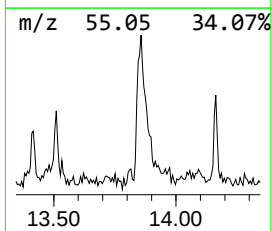
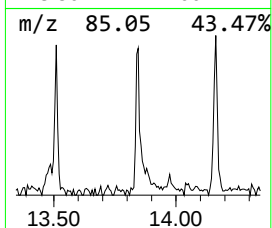
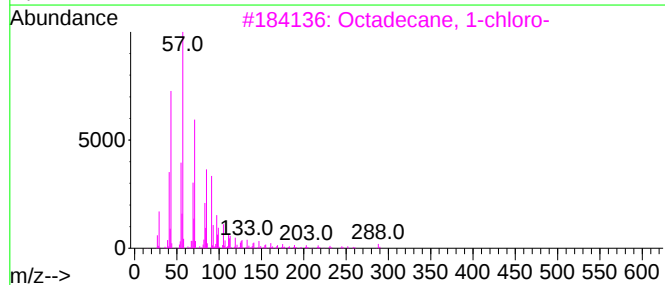
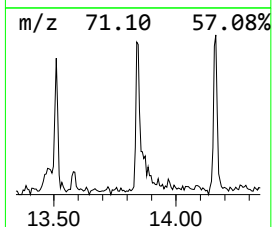
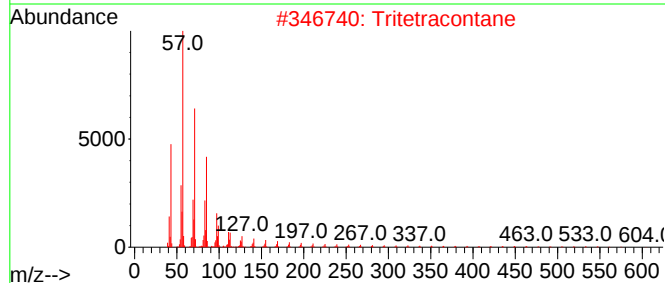
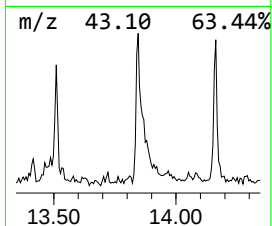
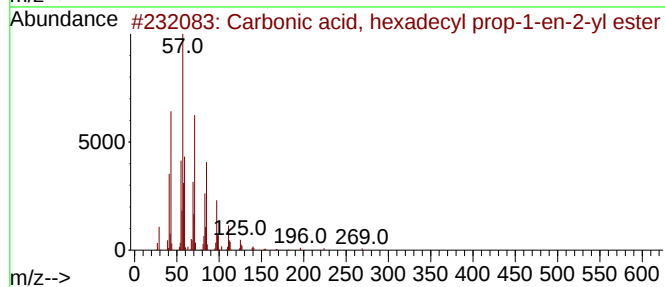
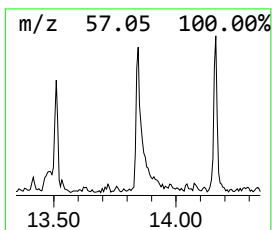
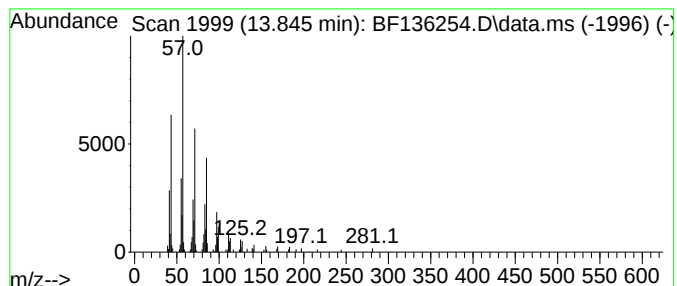
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Peak Number 5 Carbonic acid, hexadecyl pr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	5.87 ng	190678	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	91
2			Tritetracontane	605	C43H88	007098-21-7	91
3			Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	91
4			Carbonic acid, tridecyl vinyl ester	270	C16H30O3	1000382-54-7	91
5			Tetratetracontane	619	C44H90	007098-22-8	91



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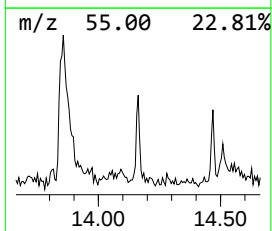
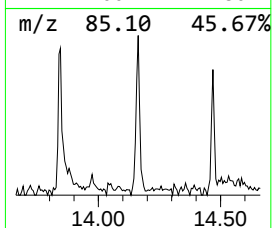
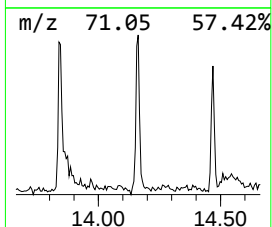
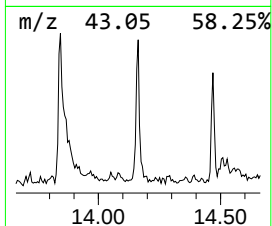
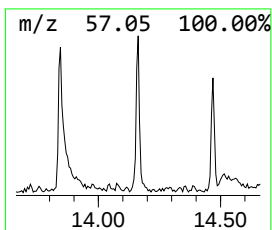
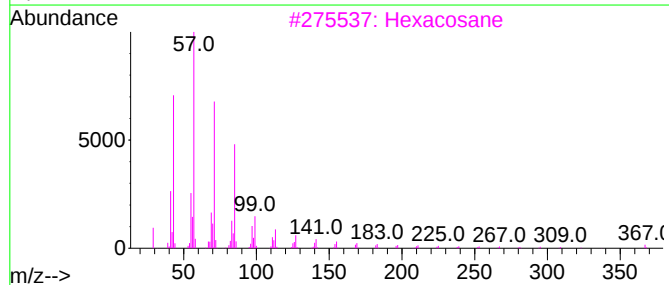
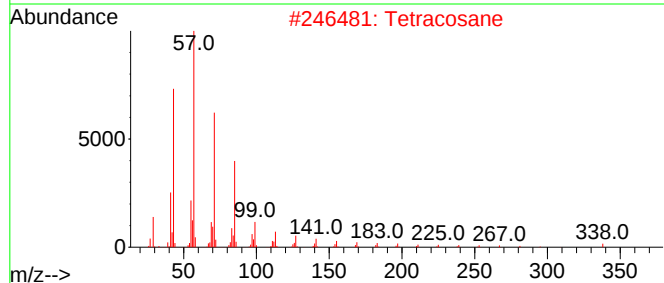
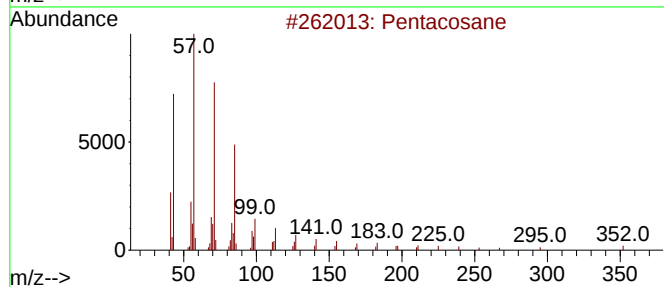
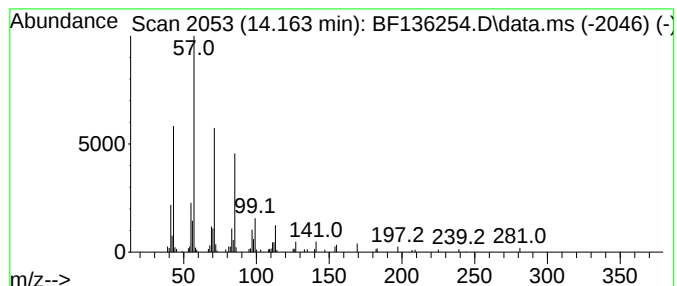
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.163	2.47 ng	80376	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	91
2			Tetracosane	338	C24H50	000646-31-1	90
3			Hexacosane	366	C26H54	000630-01-3	90
4			Heptadecane	240	C17H36	000629-78-7	90
5			Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112823\
Data File : BF136254.D
Acq On : 28 Nov 2023 17:53
Operator : CG\JU
Sample : 05468-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-9

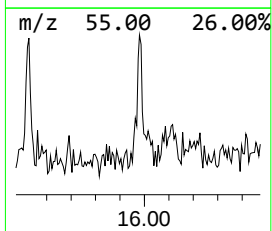
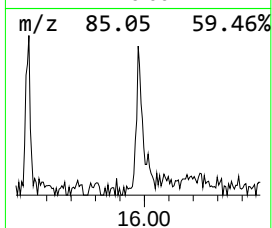
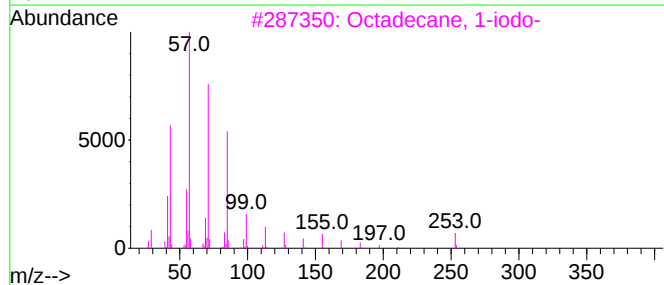
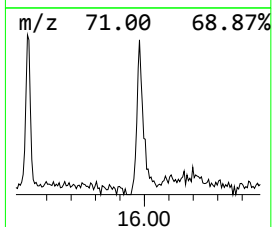
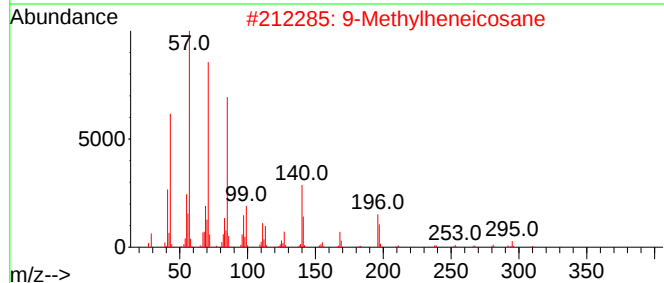
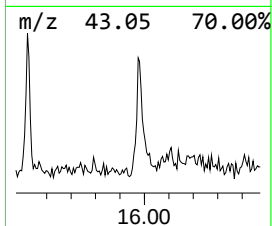
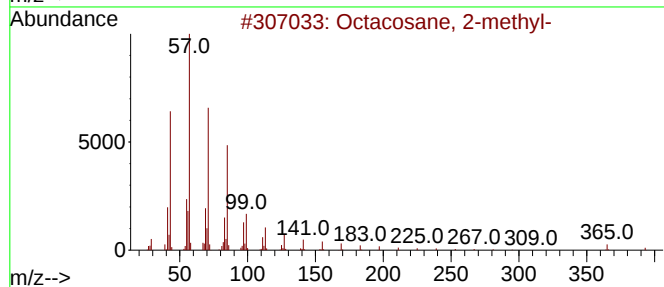
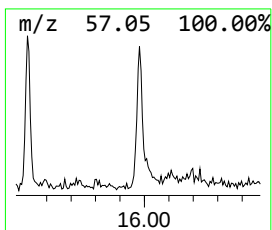
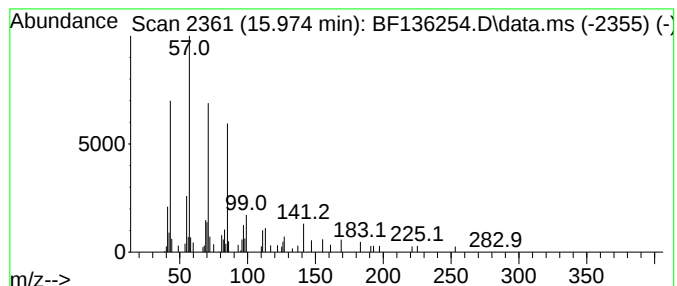
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.974	2.54 ng	80375	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
2			9-Methylheneicosane	310	C22H46	070475-51-3	86
3			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
4			Triacontane	422	C30H62	000638-68-6	86
5			Pentacosane	352	C25H52	000629-99-2	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112823\
Data File : BF136254.D
Acq On : 28 Nov 2023 17:53
Operator : CG\JU
Sample : 05468-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-9

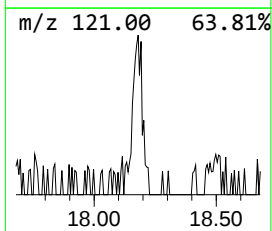
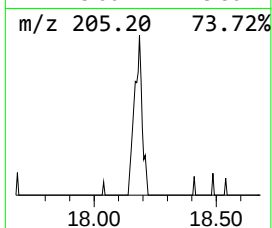
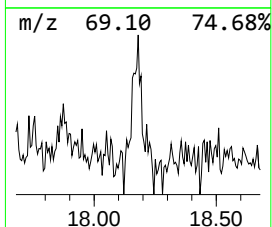
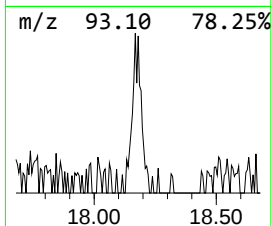
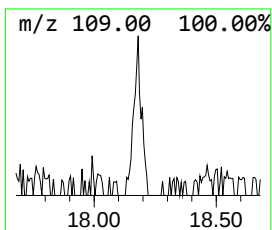
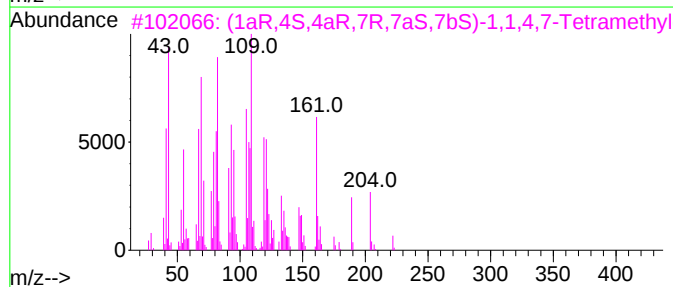
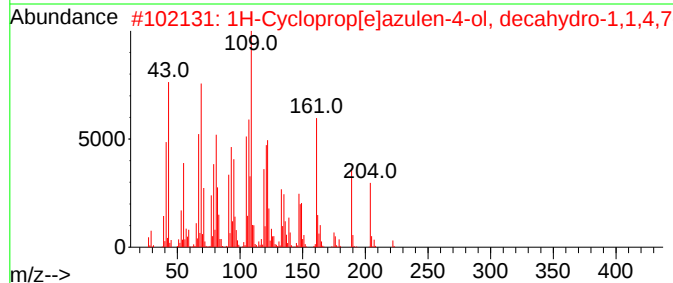
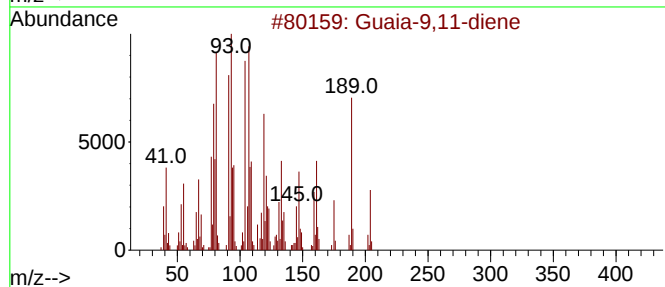
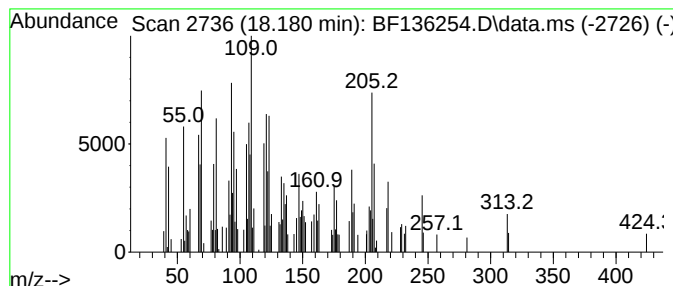
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Guaia-9,11-diene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.180	3.76 ng	118851	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Guaia-9,11-diene	204	C15H24	1000374-19-8	52
2			1H-Cycloprop[e]azulen-4-ol, deca...	222	C15H26O	000552-02-3	43
3			(1aR,4S,4aR,7R,7aS,7bS)-1,1,4,7-...	222	C15H26O	088728-58-9	41
4			4-(1,3,3-Trimethyl-bicyclo[4.1.0...	206	C14H22O	077143-31-8	35
5			Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112823\
Data File : BF136254.D
Acq On : 28 Nov 2023 17:53
Operator : CG\JU
Sample : 05468-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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...	2.122	13.6	ng	524928	1	6.804	772633	20.0
2-Pentanone, 4-...	5.051	17.3	ng	668593	1	6.804	772633	20.0
n-Hexadecanoic ...	11.869	6.7	ng	402079	4	11.328	1200800	20.0
Octadecanoic acid	12.657	7.2	ng	234647	5	13.980	649590	20.0
Carbonic acid, ...	13.845	5.9	ng	190678	5	13.980	649590	20.0
Pentacosane	14.163	2.5	ng	80376	5	13.980	649590	20.0
Octacosane, 2-m...	15.974	2.5	ng	80375	6	15.457	632127	20.0
Guaia-9,11-diene	18.180	3.8	ng	118851	6	15.457	632127	20.0