

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
 Data File : BF125180.D
 Acq On : 24 Aug 2021 12:13
 Operator : JU/CG
 Sample : PB138616BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB138616BL

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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125180.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.257	20	29	36	rVB	86265	125289	2.91%	0.448%
2	5.151	517	521	531	rVB	120933	154548	3.59%	0.552%
3	5.540	581	587	590	rBV	4166517	4063429	94.34%	14.518%
4	6.540	751	757	760	rBV	3724042	3898325	90.51%	13.928%
5	6.916	817	821	824	rBV	1036126	847553	19.68%	3.028%
6	7.475	911	916	919	rBV	2521066	2522494	58.56%	9.013%
7	8.198	1034	1039	1042	rBV	1169667	1058364	24.57%	3.781%
8	9.269	1216	1221	1225	rBV	4407160	4307217	100.00%	15.389%
9	9.951	1333	1337	1340	rBV	1366457	1100435	25.55%	3.932%
10	10.739	1467	1471	1474	rBV	2977829	2537492	58.91%	9.066%
11	11.439	1586	1590	1593	rBV	1302914	1047565	24.32%	3.743%
12	11.951	1673	1677	1688	rBV3	33368	46234	1.07%	0.165%
13	13.027	1855	1860	1863	rBV	4237427	3856977	89.55%	13.781%
14	14.074	2035	2038	2042	rBV	866028	795223	18.46%	2.841%
15	14.857	2166	2171	2175	rBV2	43226	45511	1.06%	0.163%
16	15.210	2226	2231	2234	rVB	66516	82247	1.91%	0.294%
17	15.574	2288	2293	2296	rBV	660001	810570	18.82%	2.896%
18	16.051	2369	2374	2379	rVB	104462	150611	3.50%	0.538%
19	16.574	2457	2463	2470	rBV2	99619	183540	4.26%	0.656%
20	17.192	2562	2568	2574	rBV2	63879	125927	2.92%	0.450%
21	17.921	2686	2692	2703	rVB3	56419	134833	3.13%	0.482%
22	18.792	2832	2840	2847	rBV6	33724	93896	2.18%	0.335%

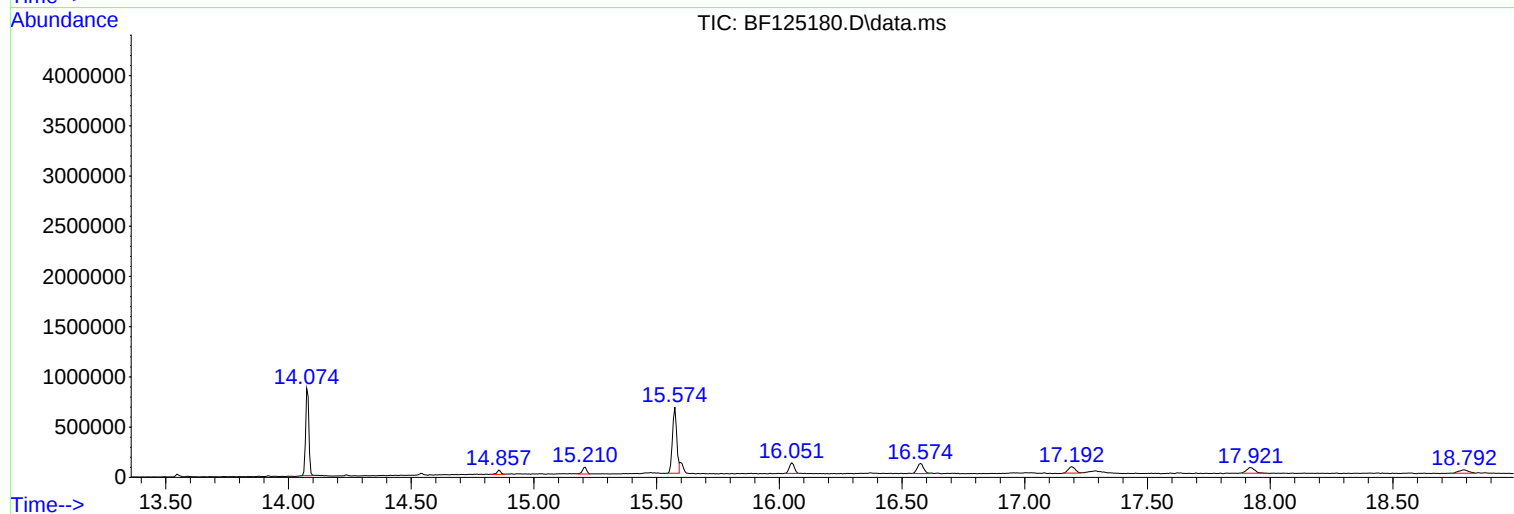
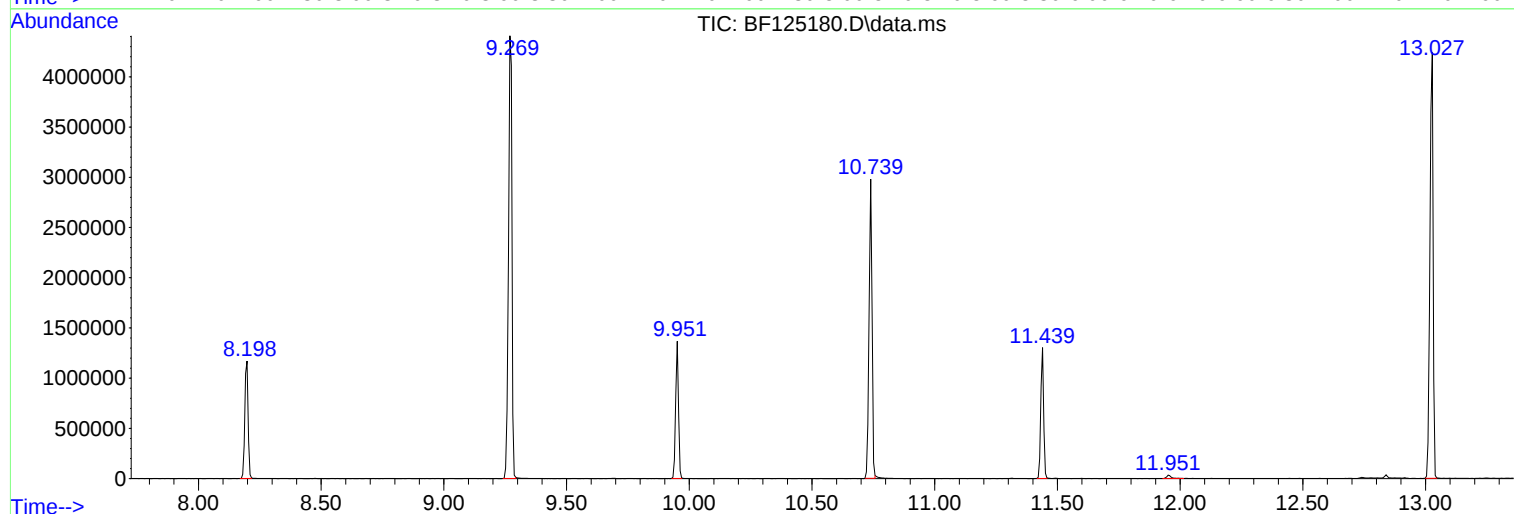
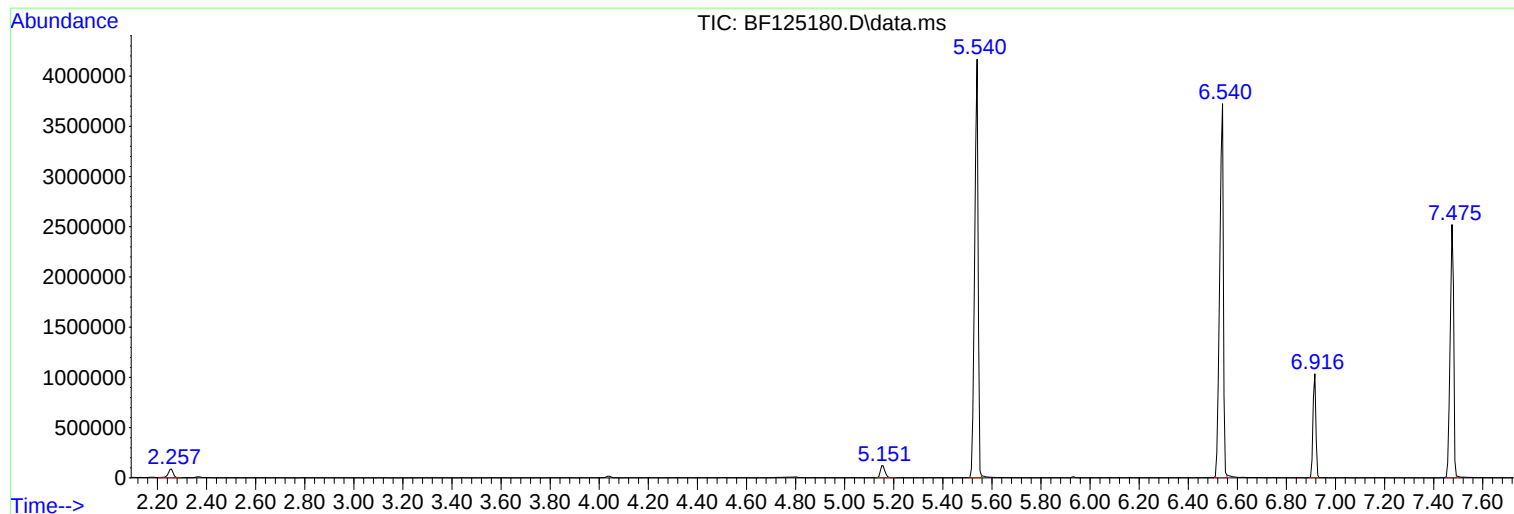
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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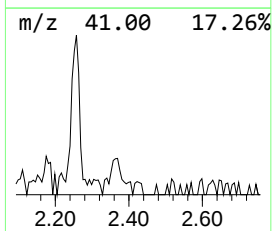
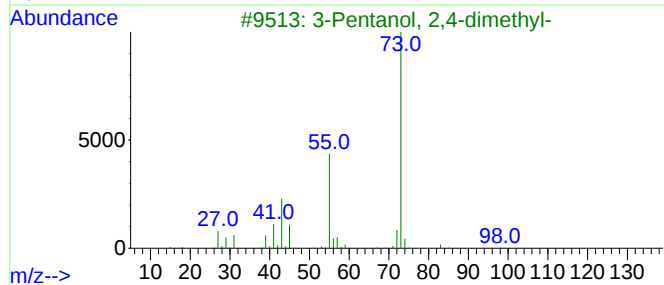
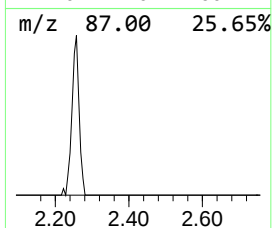
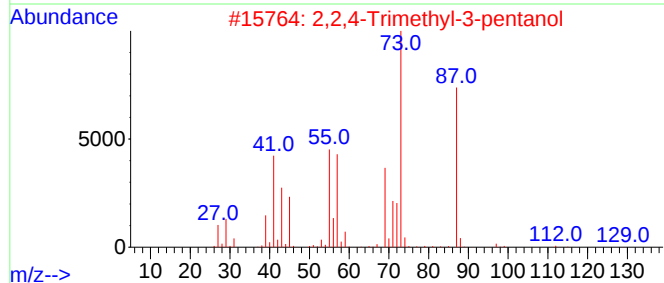
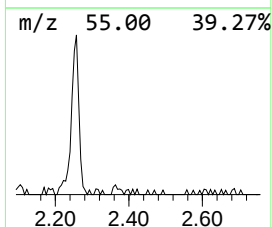
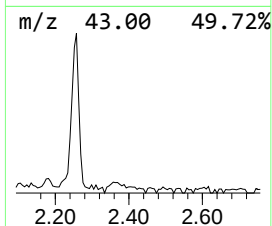
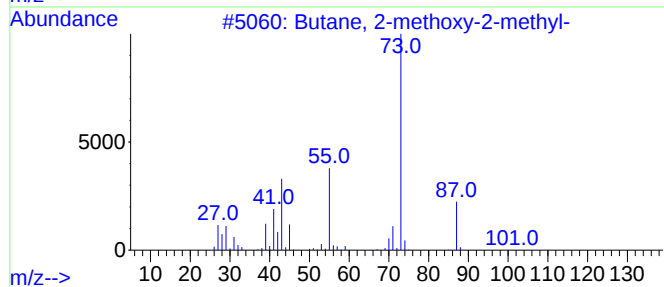
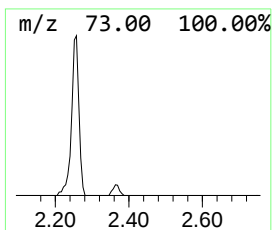
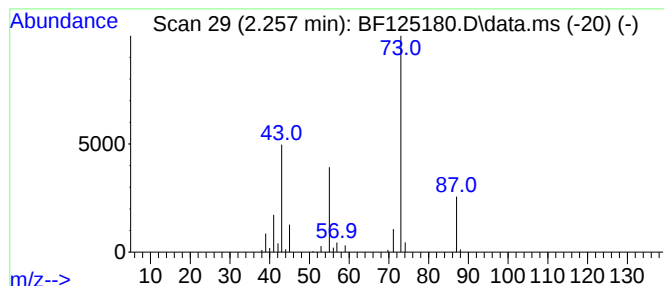
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.257	2.96 ng	125289	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	36
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	28
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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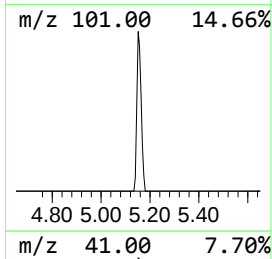
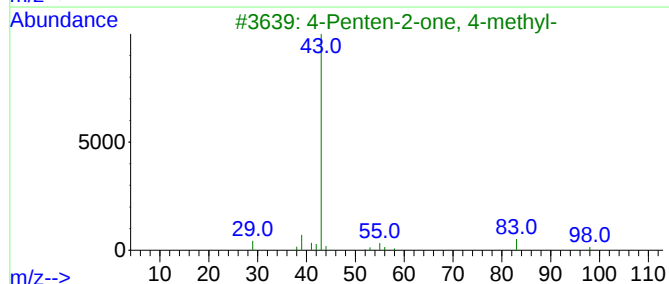
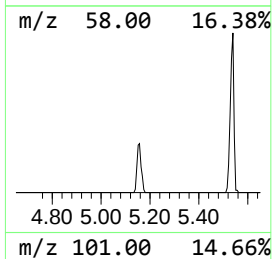
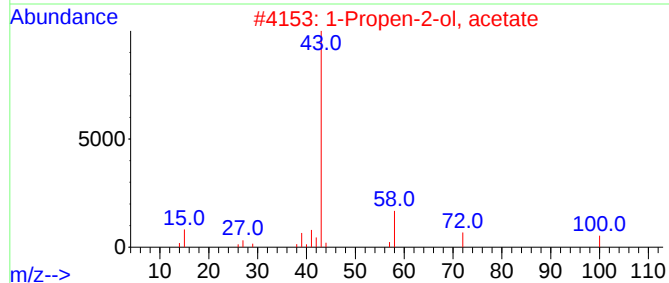
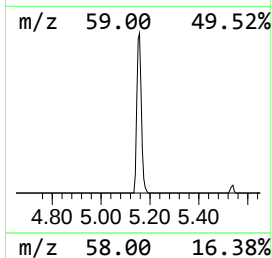
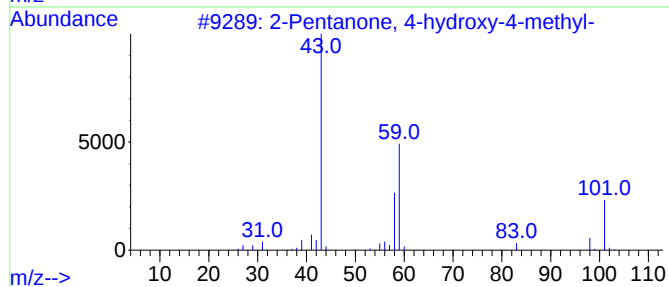
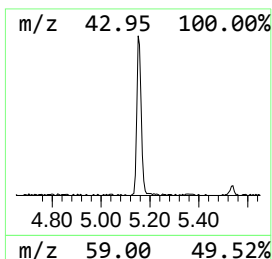
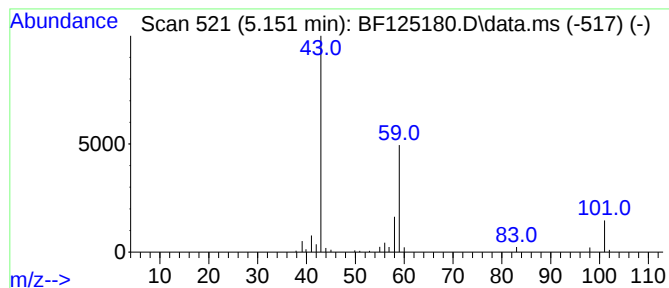
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.151	3.65 ng	154548	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5			Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7



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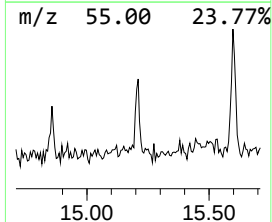
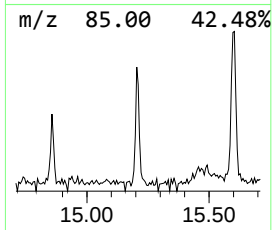
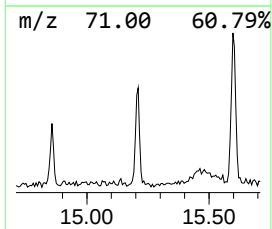
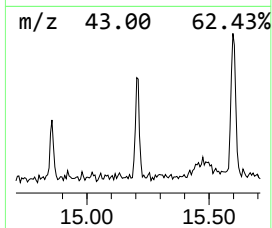
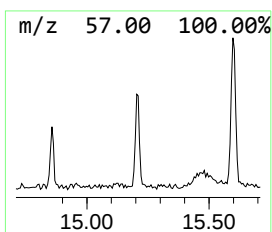
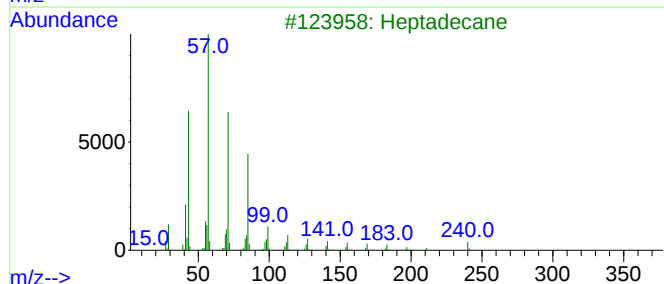
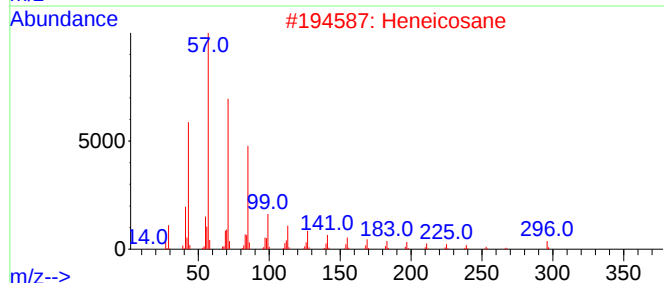
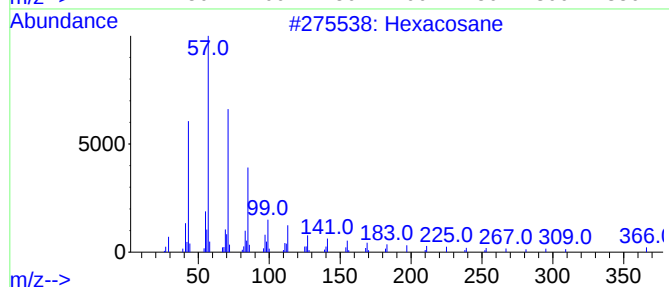
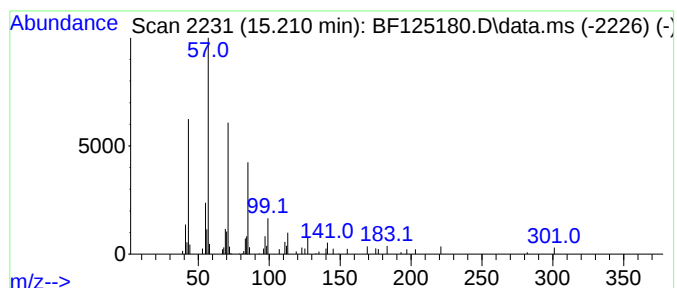
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Peak Number 3 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.210	2.03 ng	82247	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Heptadecane	240	C17H36	000629-78-7	91
4			Octadecane	254	C18H38	000593-45-3	91
5			Octacosane	394	C28H58	000630-02-4	90



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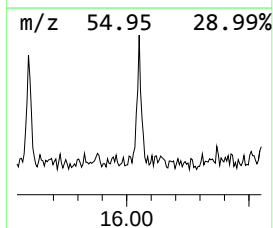
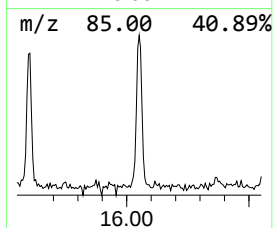
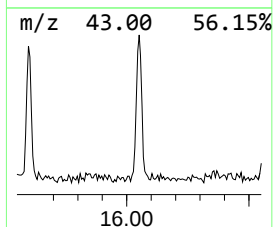
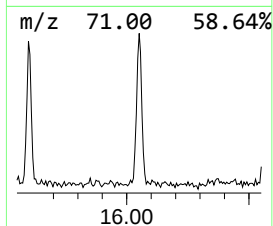
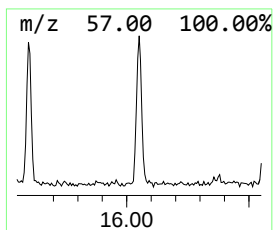
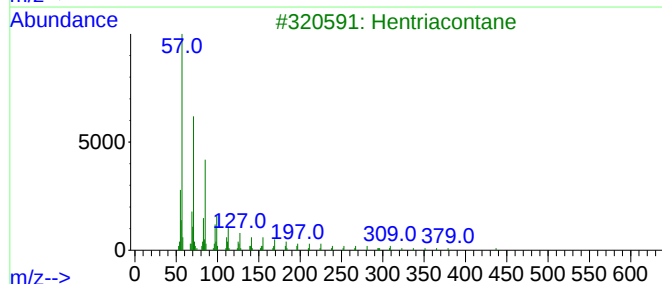
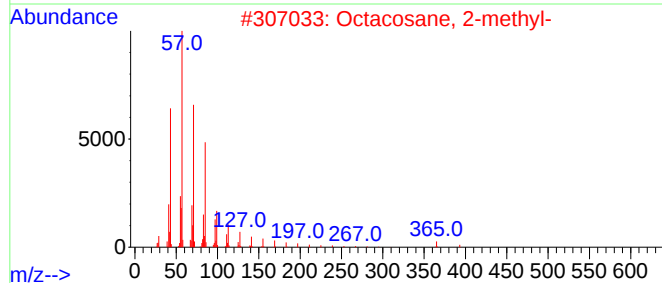
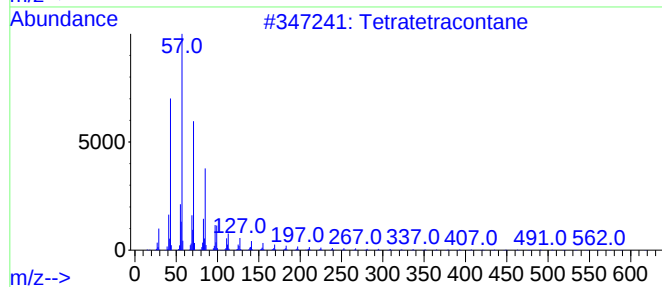
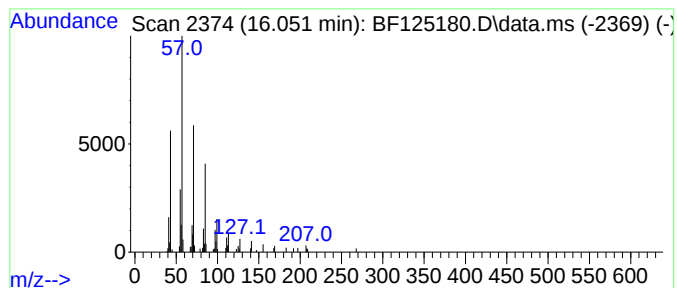
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Peak Number 4 Tetratetracontane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.051	3.72 ng	150611	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Hentriacontane	437	C31H64	000630-04-6	91
4			Nonadecane	268	C19H40	000629-92-5	91
5			triacontane	422	C30H62	000638-68-6	91



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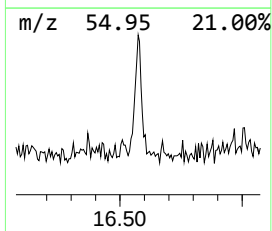
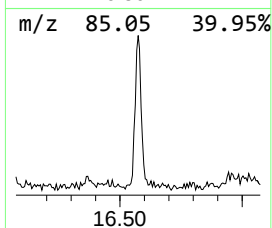
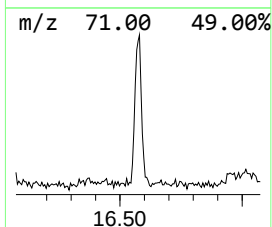
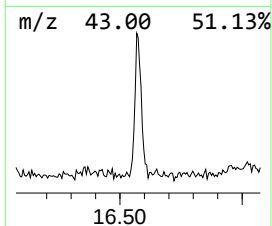
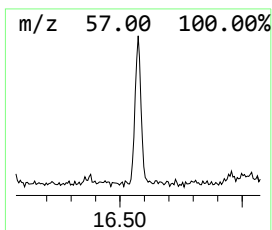
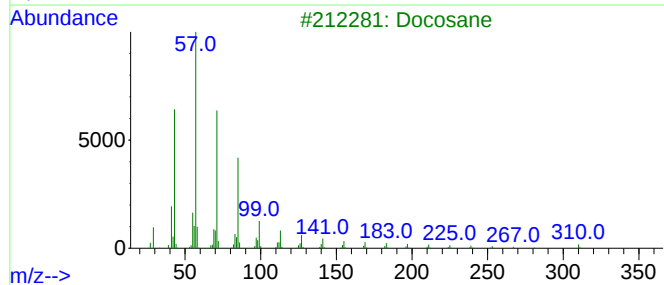
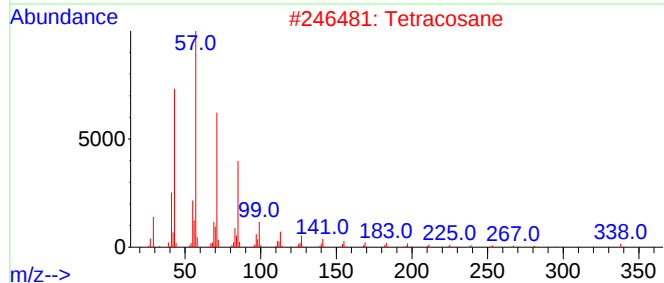
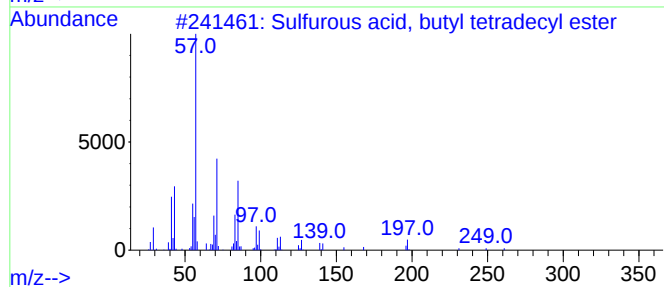
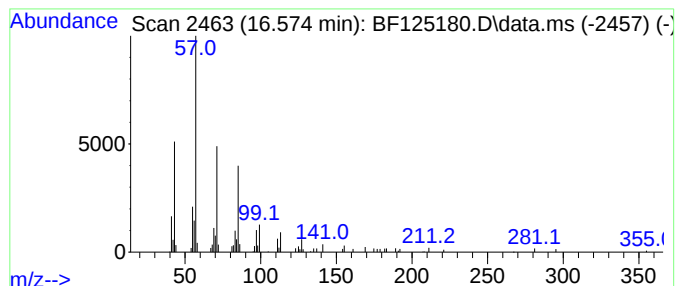
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Sulfurous acid, butyl tetra... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.574	4.53 ng	183540	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	90
2			Tetracosane	338	C24H50	000646-31-1	87
3			Docosane	310	C22H46	000629-97-0	86
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	83
5			Heneicosane	296	C21H44	000629-94-7	83



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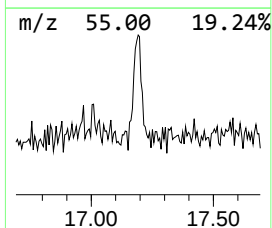
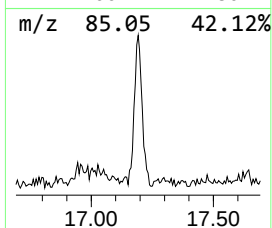
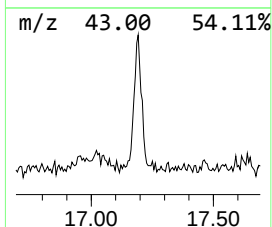
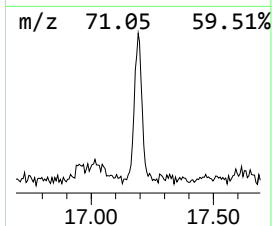
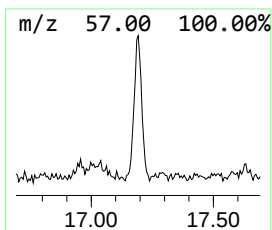
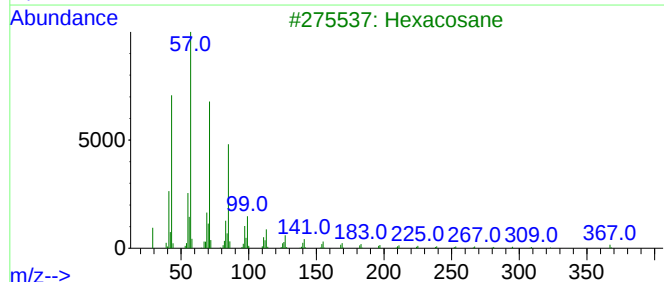
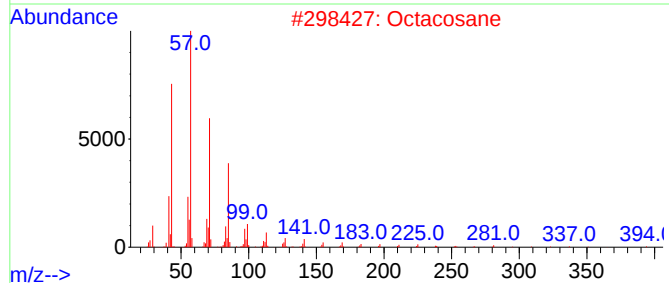
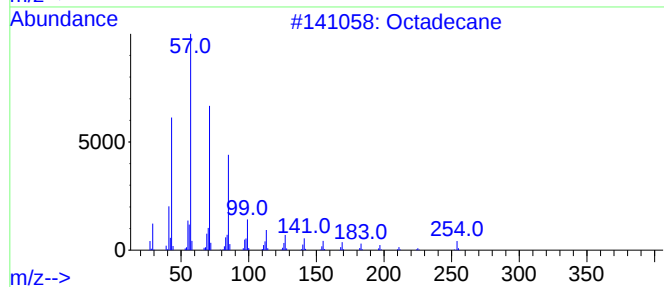
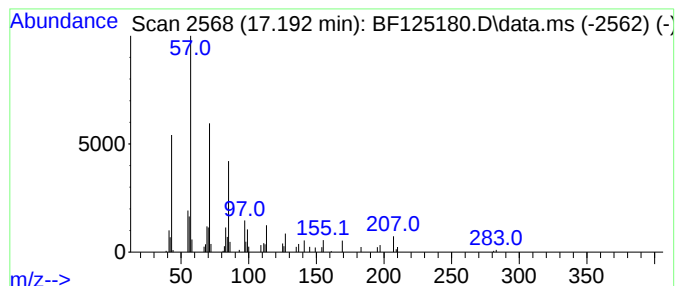
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.192	3.11 ng	125927	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	87
2			Octacosane	394	C28H58	000630-02-4	87
3			Hexacosane	366	C26H54	000630-01-3	87
4			Pentacosane	352	C25H52	000629-99-2	87
5			Heptadecane	240	C17H36	000629-78-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
Data File : BF125180.D
Acq On : 24 Aug 2021 12:13
Operator : JU/CG
Sample : PB138616BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB138616BL

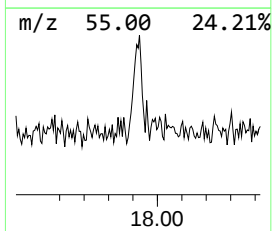
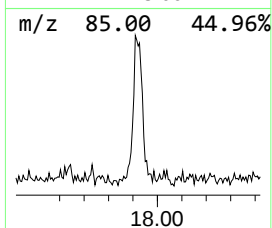
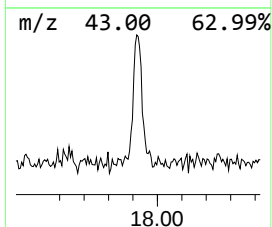
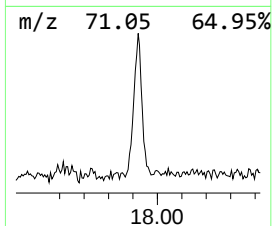
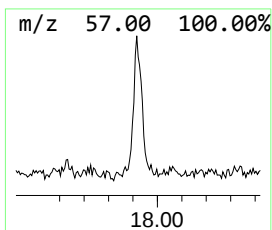
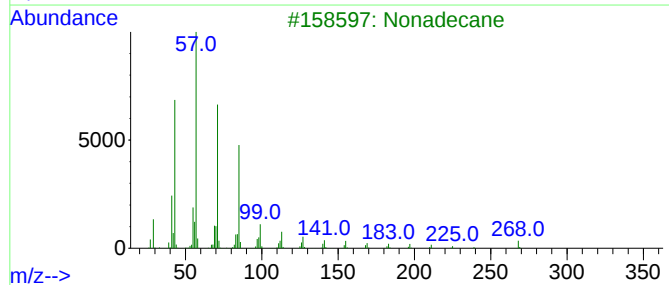
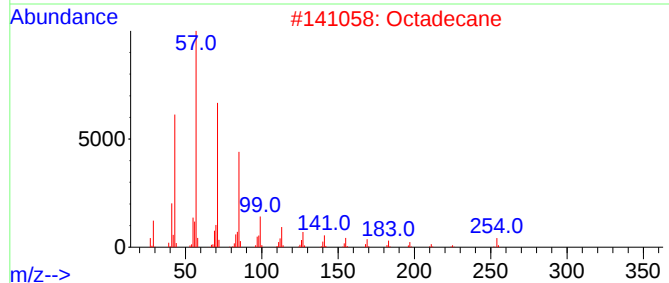
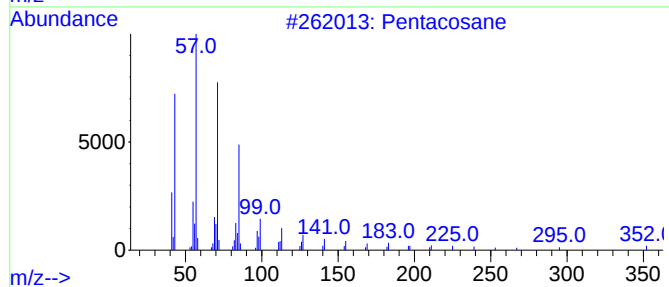
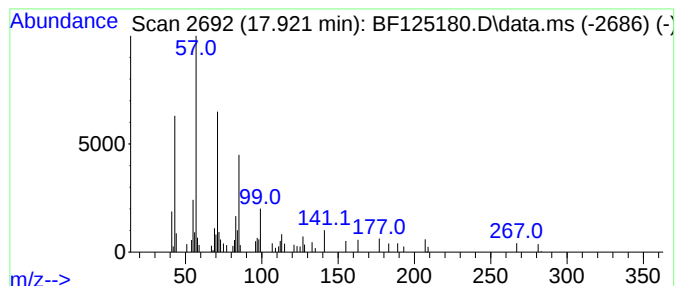
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.921	3.33 ng	134833	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	68
2			Octadecane	254	C18H38	000593-45-3	64
3			Nonadecane	268	C19H40	000629-92-5	58
4			Heneicosane	296	C21H44	000629-94-7	58
5			Heptadecane	240	C17H36	000629-78-7	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
Data File : BF125180.D
Acq On : 24 Aug 2021 12:13
Operator : JU/CG
Sample : PB138616BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB138616BL

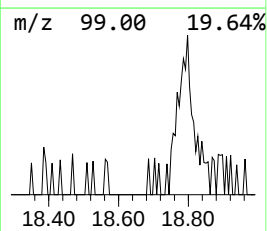
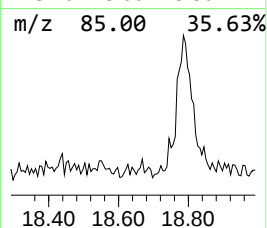
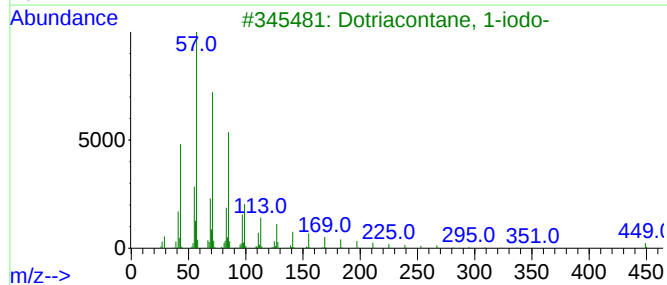
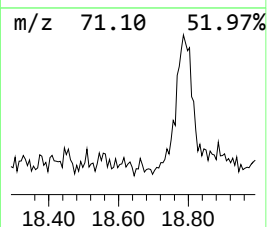
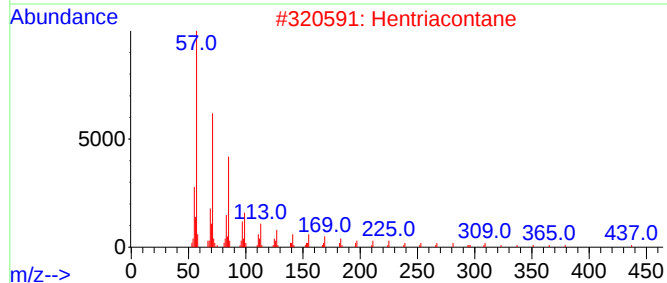
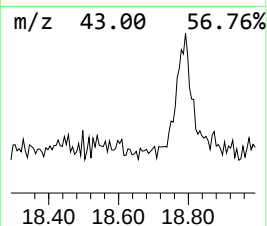
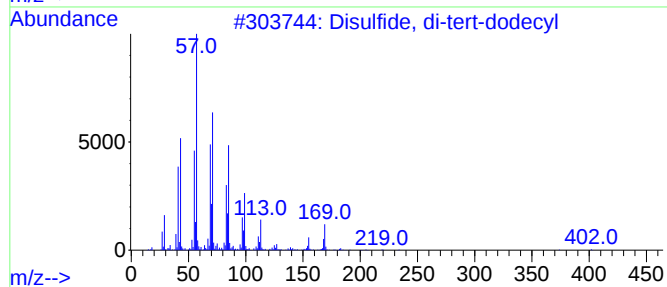
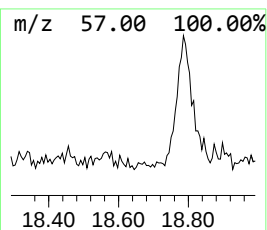
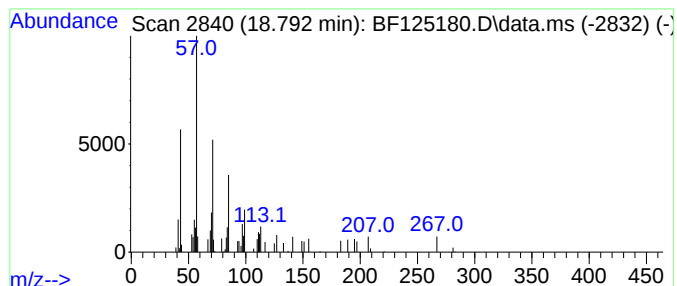
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Disulfide, di-tert-dodecyl Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.792	2.32 ng	93896	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	90
2			Hentriacontane	437	C31H64	000630-04-6	83
3			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	72
4			Nonacosane	408	C29H60	000630-03-5	72
5			Tetratetracontane	619	C44H90	007098-22-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
Data File : BF125180.D
Acq On : 24 Aug 2021 12:13
Operator : JU/CG
Sample : PB138616BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB138616BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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
Butane, 2-metho...	2.257	3.0	ng	125289	1	6.916	847553	20.0
2-Pentanone, 4-...	5.151	3.6	ng	154548	1	6.916	847553	20.0
Hexacosane	15.210	2.0	ng	82247	6	15.574	810570	20.0
Tetratetracontane	16.051	3.7	ng	150611	6	15.574	810570	20.0
Sulfurous acid,...	16.574	4.5	ng	183540	6	15.574	810570	20.0
Octadecane	17.192	3.1	ng	125927	6	15.574	810570	20.0
Pentacosane	17.921	3.3	ng	134833	6	15.574	810570	20.0
Disulfide, di-t...	18.792	2.3	ng	93896	6	15.574	810570	20.0