

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052922\
 Data File : BP010622.D
 Acq On : 29 May 2022 16:54
 Operator : CG/JU
 Sample : N2932-24
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 P023-SS001-0006-01

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_P\Methods\8270E-BP052822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP010622.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.452	395	402	419	rBV	2477401	3682434	19.11%	6.204%
2	7.040	663	672	690	rBV	2304670	3946477	20.49%	6.649%
3	7.863	805	812	821	rBV	493844	787386	4.09%	1.327%
4	9.028	1002	1010	1024	rBV	1477614	2557252	13.27%	4.308%
5	10.663	1276	1288	1300	rBV	602994	1080996	5.61%	1.821%
6	13.122	1699	1706	1723	rBV	3277648	5123454	26.59%	8.632%
7	14.498	1933	1940	1957	rBV	860852	1363728	7.08%	2.298%
8	15.992	2186	2194	2203	rBV	2617497	3846664	19.97%	6.481%
9	17.257	2402	2409	2414	rBV	1000536	1480424	7.68%	2.494%
10	18.145	2555	2560	2569	rBV	161506	256258	1.33%	0.432%
11	19.810	2838	2843	2855	rBV	5450498	6621349	34.37%	11.156%
12	21.051	3049	3054	3061	rBV3	517892	765054	3.97%	1.289%
13	21.251	3084	3088	3094	rBV	610120	685404	3.56%	1.155%
14	21.339	3098	3103	3109	rBV	1187769	1576235	8.18%	2.656%
15	21.463	3117	3124	3138	rBV	12653324	19264904	100.00%	32.457%
16	21.774	3175	3177	3183	rVB	154392	193734	1.01%	0.326%
17	23.010	3384	3387	3391	rVB	219523	299117	1.55%	0.504%
18	23.751	3508	3513	3521	rVB2	748860	1521351	7.90%	2.563%
19	24.374	3614	3619	3627	rVB	332813	673655	3.50%	1.135%
20	24.468	3630	3635	3650	rVB	593949	1469056	7.63%	2.475%
21	26.821	4028	4035	4050	rVB3	698744	2159929	11.21%	3.639%

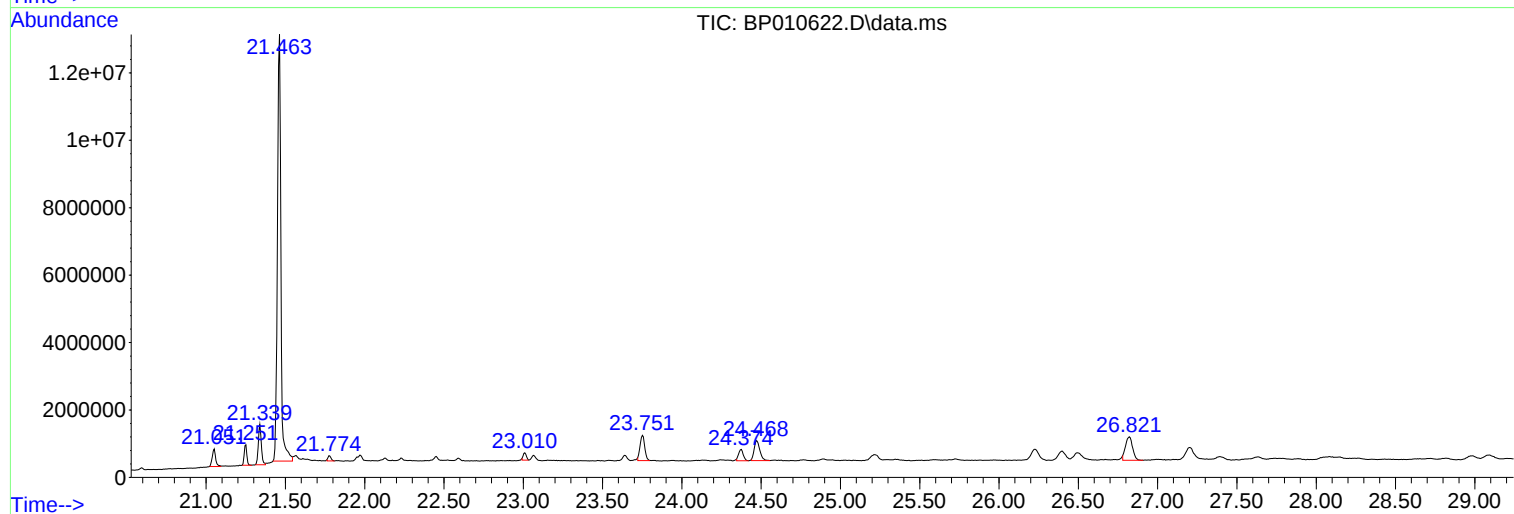
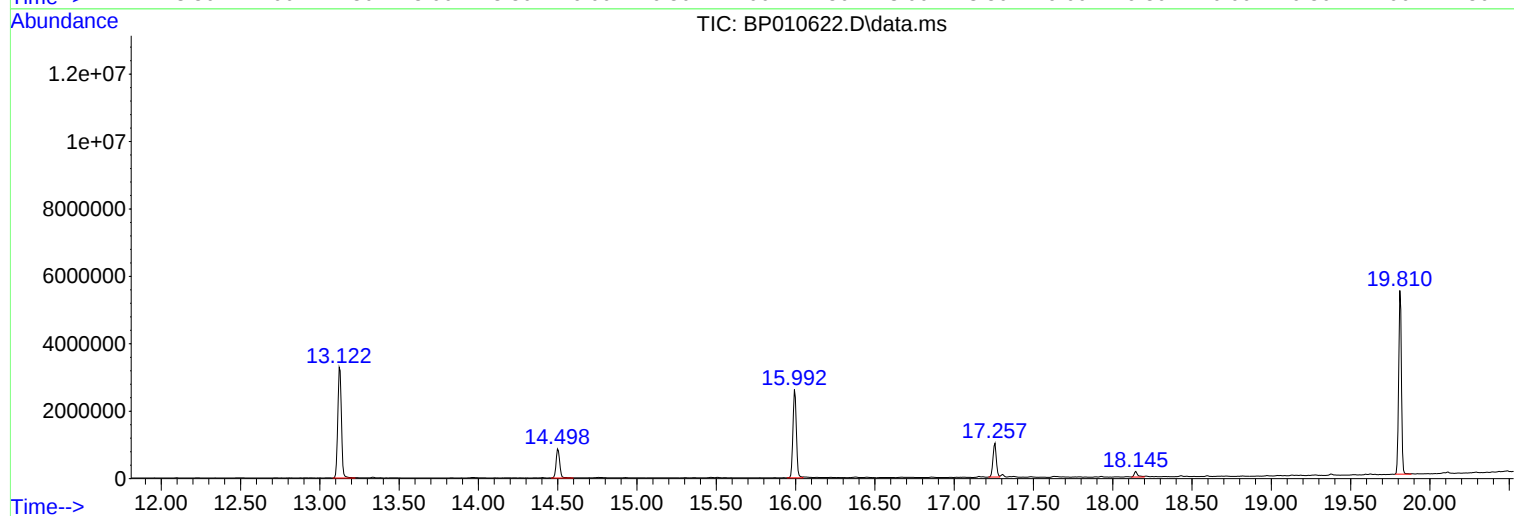
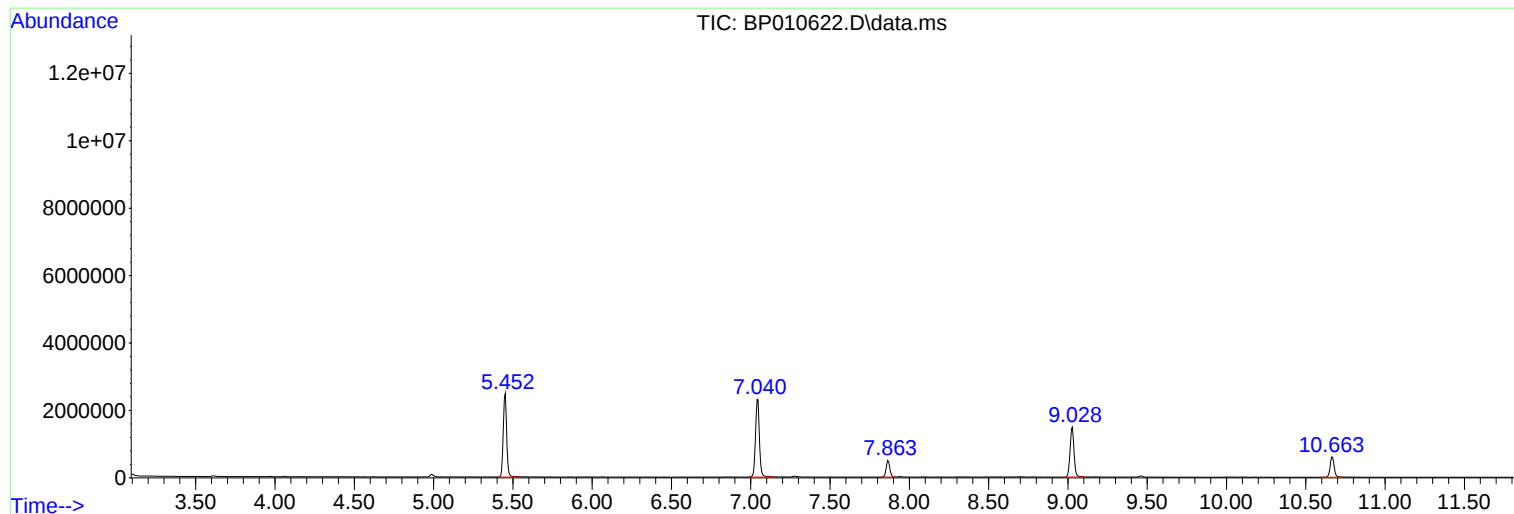
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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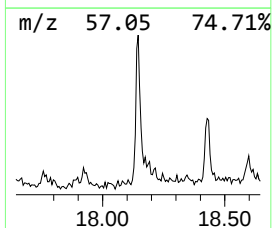
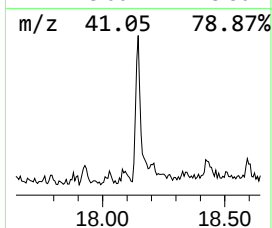
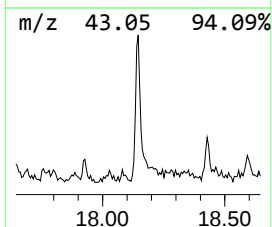
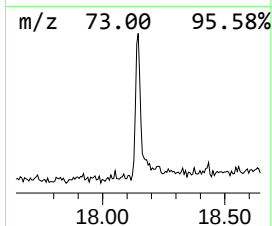
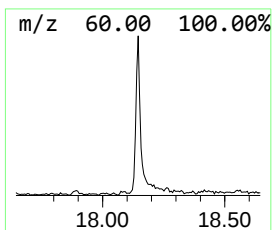
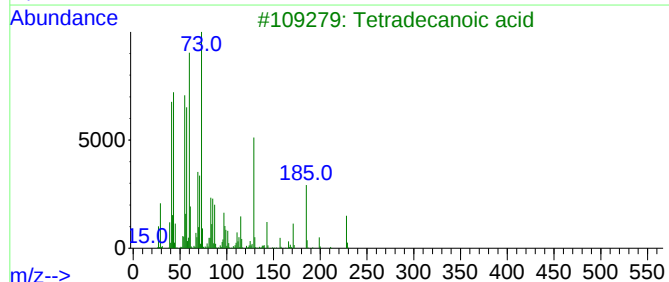
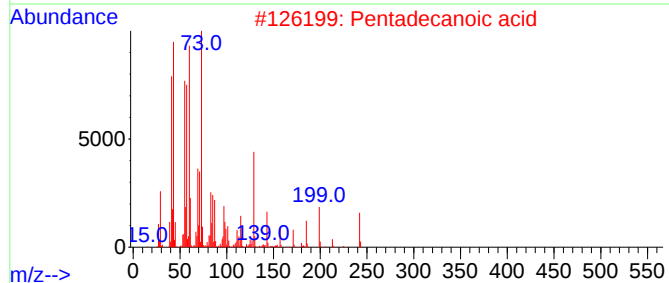
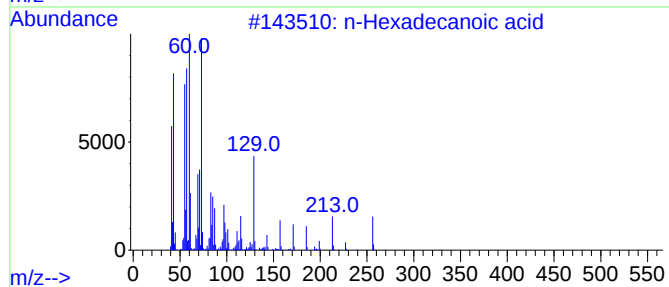
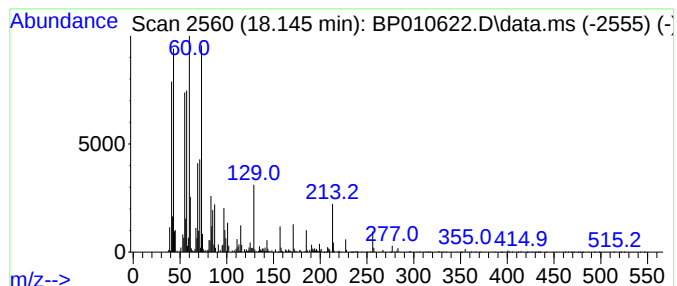
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.145	3.46 ng	256258	Phenanthrene-d10	17.257

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	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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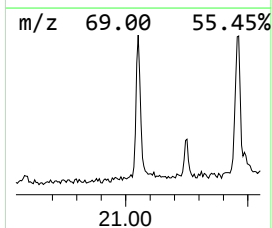
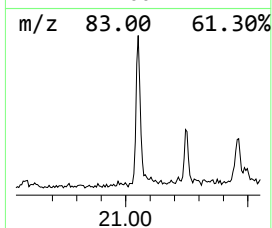
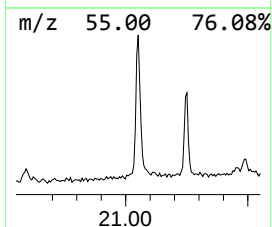
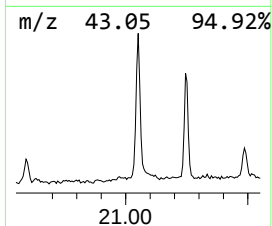
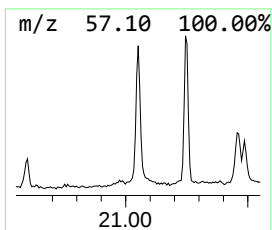
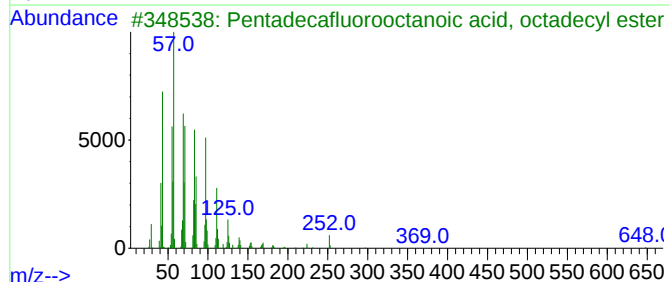
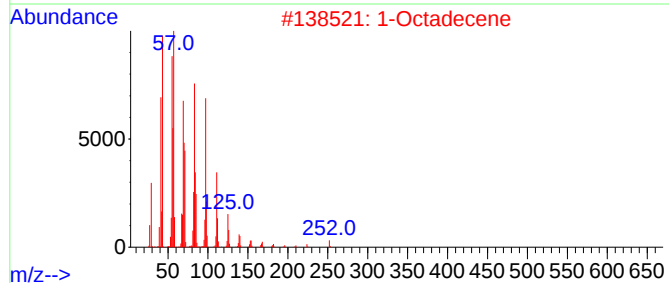
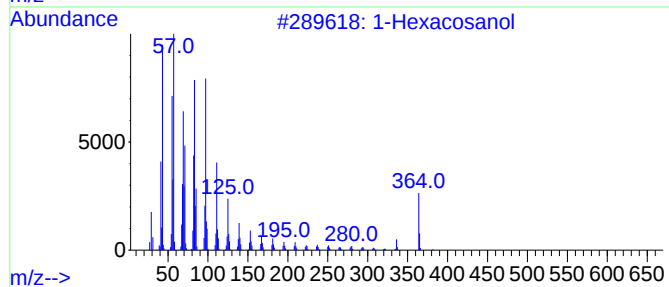
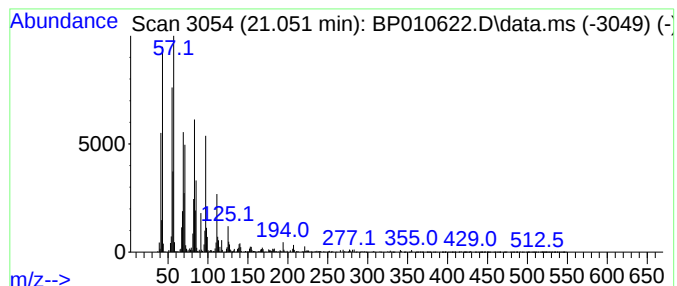
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1-Hexacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.051	9.71 ng	765054	Chrysene-d12	21.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol			382	C26H54O	000506-52-5	94
2	1-Octadecene			252	C18H36	000112-88-9	94
3	Pentadecafluorooctanoic acid, oc...			666	C26H37F15O2	1000406-04-8	94
4	Heptafluorobutyric acid, pentade...			424	C19H31F7O2	959261-23-5	94
5	Pentafluoropropionic acid, hepta...			402	C20H35F5O2	959218-78-1	91



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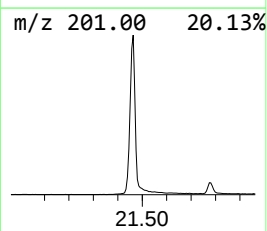
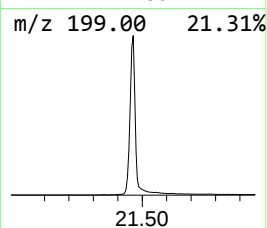
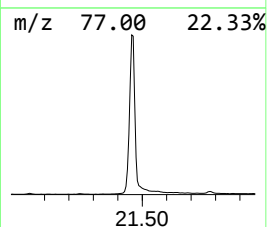
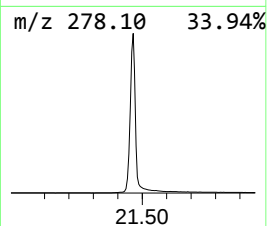
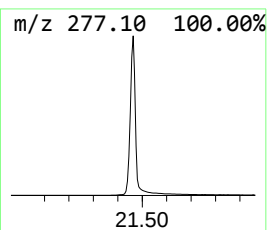
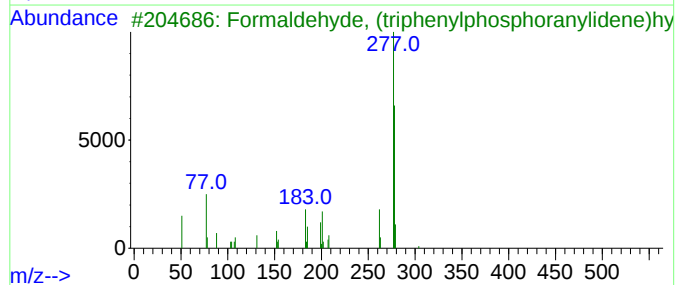
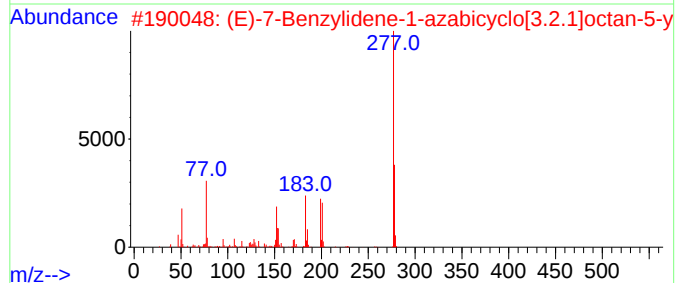
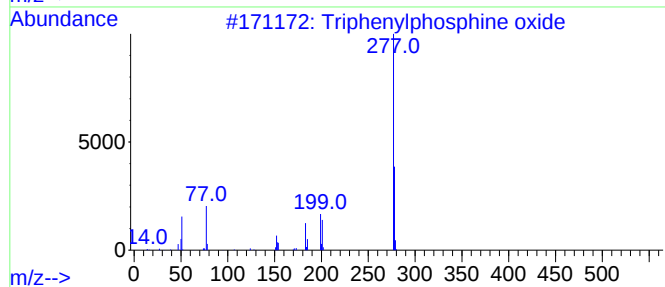
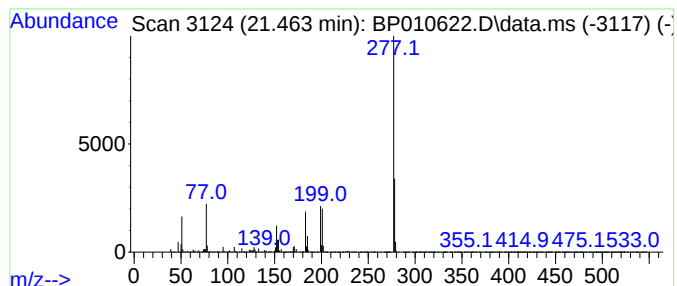
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.463	244.44 ng	19264900	Chrysene-d12	21.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	25
5			1H-Indole-3-acetic acid, 5-[(tri...	277	C14H19NO3Si	072101-35-0	23



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Misc :
ALS Vial : 11 Sample Multiplier: 1

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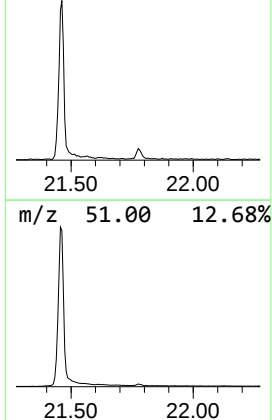
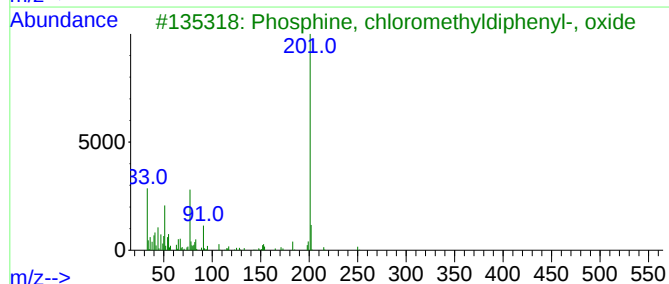
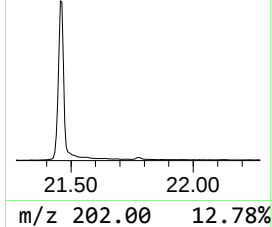
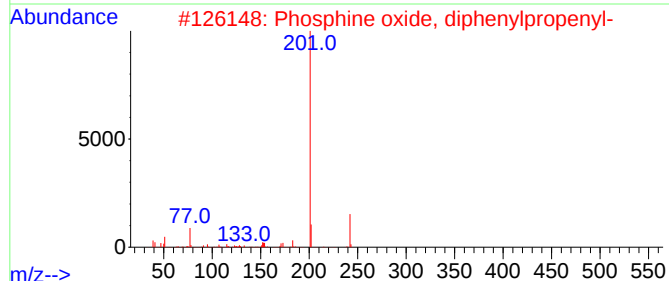
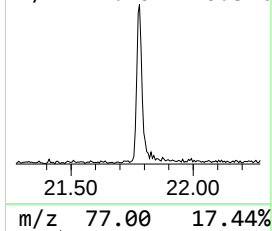
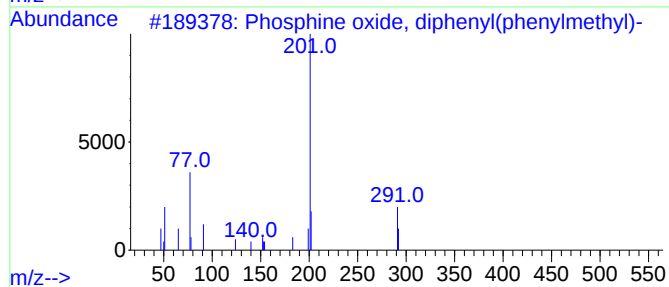
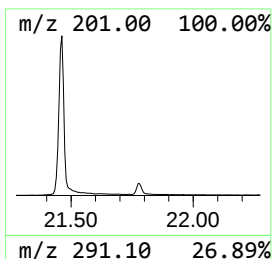
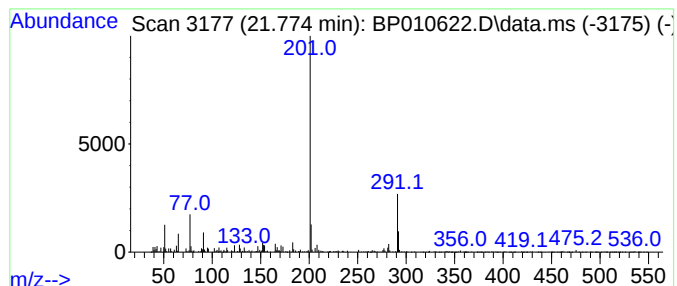
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phosphine oxide, diphenyl(p... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.774	2.46 ng	193734	Chrysene-d12	21.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phosphine oxide, diphenyl(phenyl...)	292	C19H17OP	002959-74-2	87
2			Phosphine oxide, diphenylpropenyl-	242	C15H15OP	004252-89-5	52
3			Phosphine, chloromethyldiphenyl-...	250	C13H12ClOP	001806-49-1	40
4			3H-Pyrazol-3-one, 2,4-dihydro-5-...	244	C14H16N2O2	022616-35-9	40
5			Ethyldiphenylphosphine oxide	230	C14H15OP	001733-57-9	37



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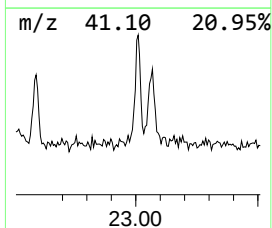
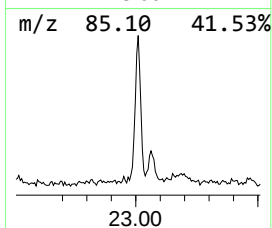
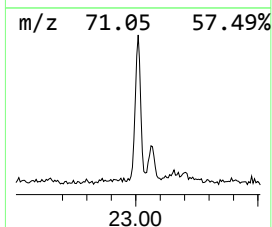
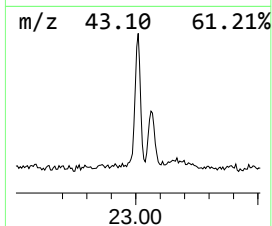
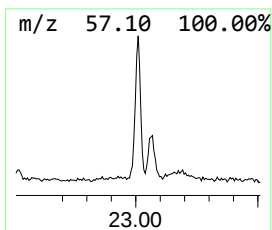
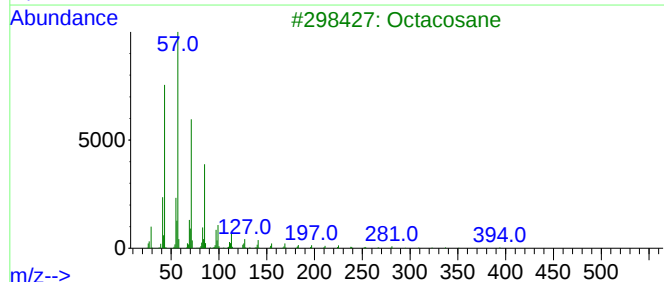
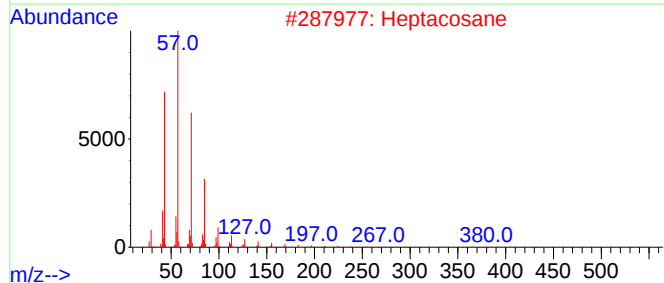
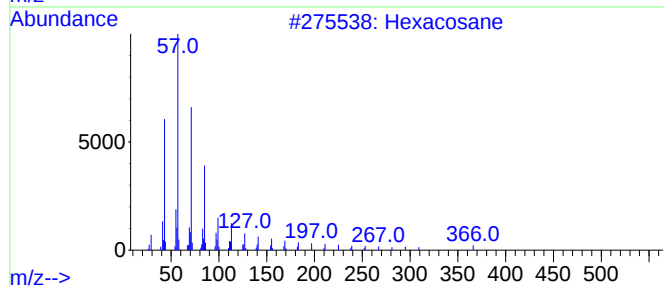
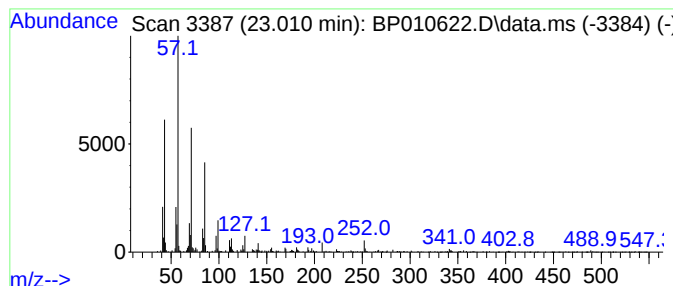
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.010	3.93 ng	299117	Perylene-d12	23.751

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Heptacosane	380	C27H56	000593-49-7	83
3			Octacosane	394	C28H58	000630-02-4	83
4			Heneicosane	296	C21H44	000629-94-7	83
5			Undecane, 2,10-dimethyl-	184	C13H28	017301-27-8	80



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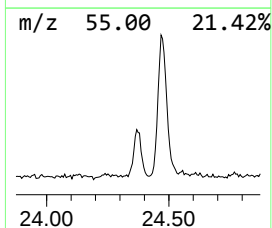
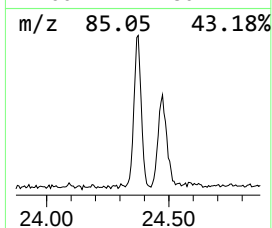
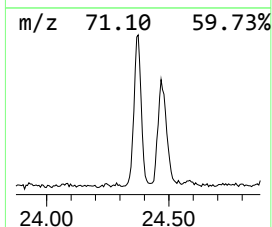
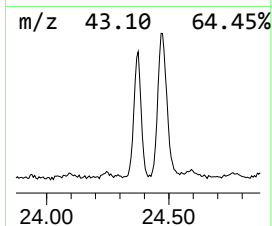
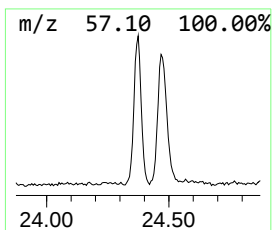
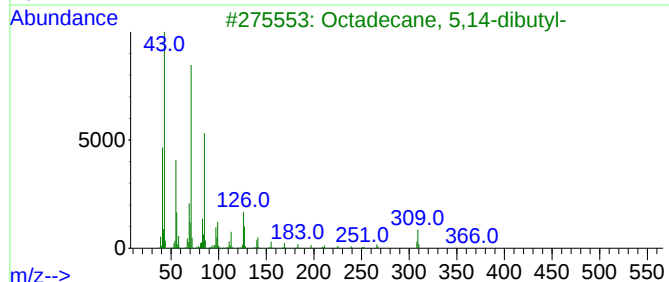
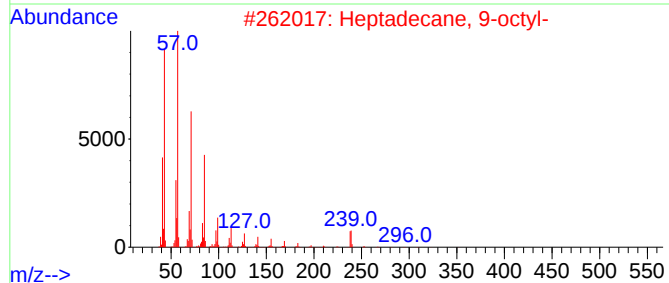
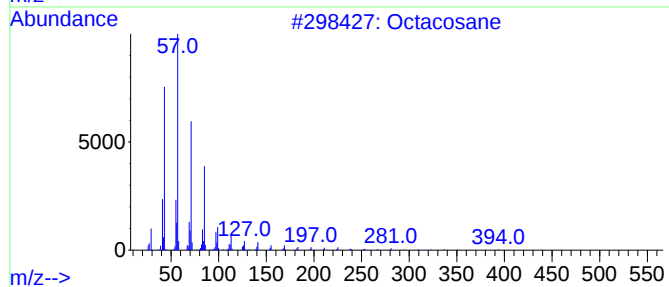
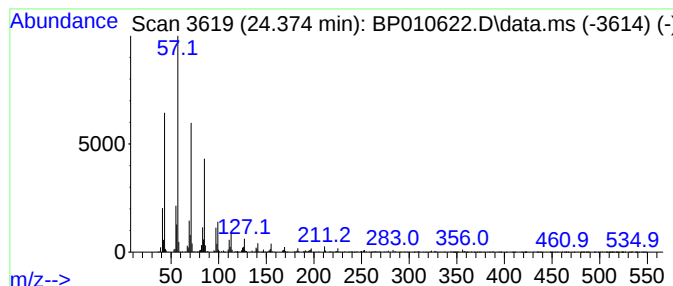
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.374	8.86 ng	673655	Perylene-d12	23.751

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	98
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	94
3			Octadecane, 5,14-dibutyl-	366	C26H54	055282-13-8	93
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	93
5			Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052922\
Data File : BP010622.D
Acq On : 29 May 2022 16:54
Operator : CG/JU
Sample : N2932-24
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
P023-SS001-0006-01

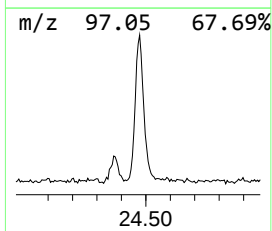
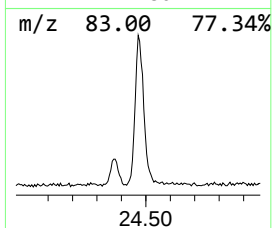
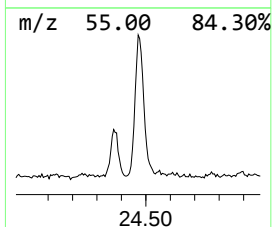
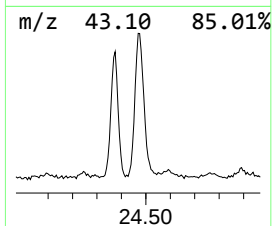
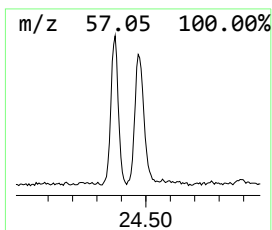
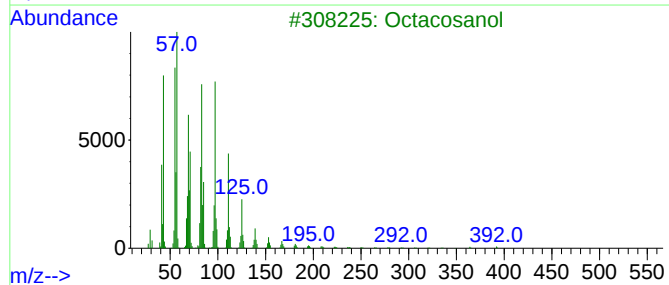
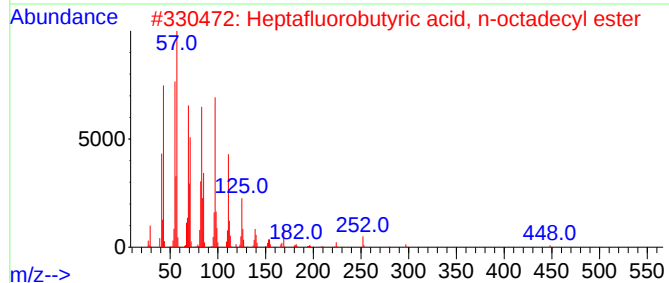
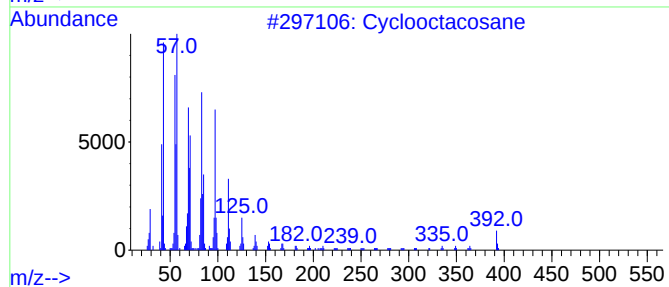
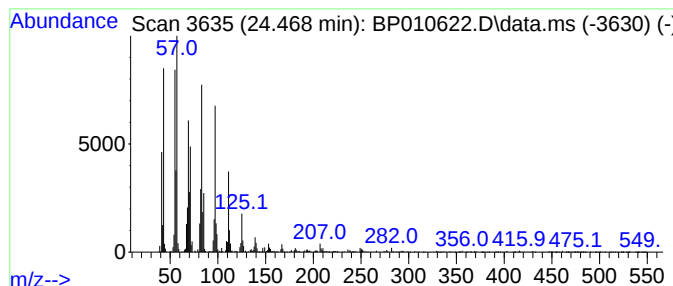
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclooctacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.468	19.31 ng	1469060	Perylene-d12	23.751

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclooctacosane	392	C28H56	000297-24-5	95
2			Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	94
3			Octacosanol	410	C28H58O	000557-61-9	94
4			1-Hexacosene	364	C26H52	018835-33-1	94
5			1-Heneicosanol	312	C21H44O	015594-90-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052922\
Data File : BP010622.D
Acq On : 29 May 2022 16:54
Operator : CG/JU
Sample : N2932-24
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
P023-SS001-0006-01

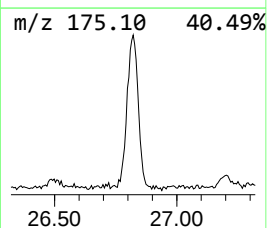
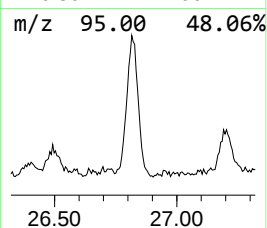
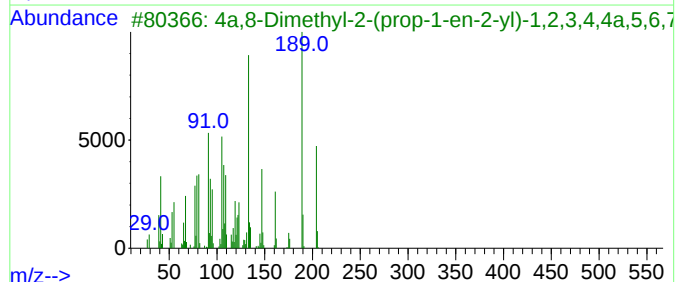
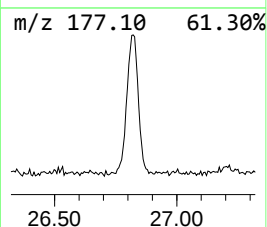
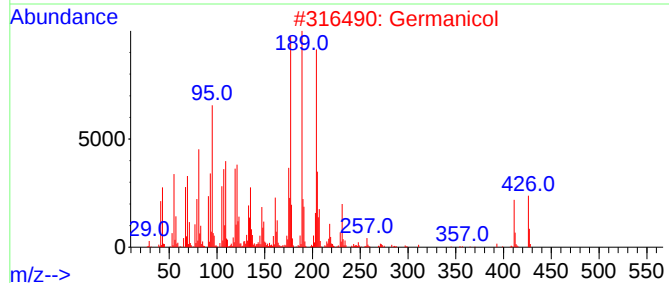
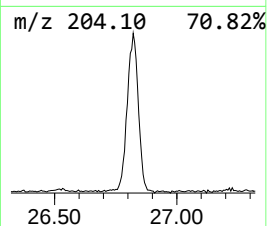
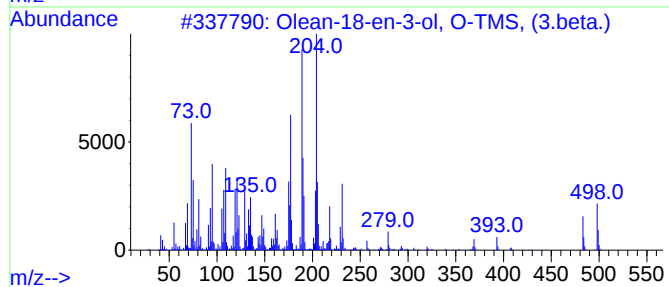
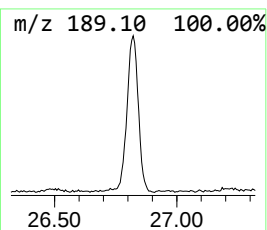
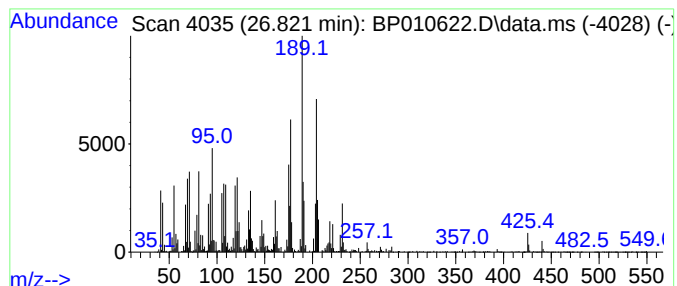
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Olean-18-en-3-ol, O-TMS, (3... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.821	28.39 ng	2159930	Perylene-d12	23.751

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Olean-18-en-3-ol, O-TMS, (3.beta.)	498	C33H58OSi	1000465-44-5	70
2			Germanicol	426	C30H50O	000465-02-1	62
3			4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	49
4			Germanicol acetate	468	C32H52O2	010483-91-7	49
5			Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	005951-61-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052922\
Data File : BP010622.D
Acq On : 29 May 2022 16:54
Operator : CG/JU
Sample : N2932-24
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
P023-SS001-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052822.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
n-Hexadecanoic ...	18.145	3.5	ng	256258	4	17.257	1480420	20.0
1-Hexacosanol	21.051	9.7	ng	765054	5	21.339	1576240	20.0
Triphenylphosph...	21.463	244.4	ng	19264900	5	21.339	1576240	20.0
Phosphine oxide...	21.774	2.5	ng	193734	5	21.339	1576240	20.0
Hexacosane	23.010	3.9	ng	299117	6	23.751	1521350	20.0
Octacosane	24.374	8.9	ng	673655	6	23.751	1521350	20.0
Cyclooctacosane	24.468	19.3	ng	1469060	6	23.751	1521350	20.0
Olean-18-en-3-o...	26.821	28.4	ng	2159930	6	23.751	1521350	20.0