

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
 Data File : BP008275.D
 Acq On : 08 Dec 2021 11:56
 Operator : CG/JU
 Sample : PB141209BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 PB141209BL

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-BP112521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008275.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.369	399	405	422	rBV	1525116	2336506	45.65%	9.913%
2	6.269	545	558	580	rVB2	64564	386223	7.55%	1.639%
3	6.969	666	677	698	rBV	1362147	2307941	45.09%	9.792%
4	7.775	807	814	823	rVB	280096	431210	8.42%	1.829%
5	8.940	1004	1012	1032	rBV	820161	1412425	27.59%	5.992%
6	9.193	1042	1055	1064	rVB4	28551	83421	1.63%	0.354%
7	10.575	1282	1290	1303	rBV	316050	563950	11.02%	2.393%
8	13.051	1703	1711	1721	rBV	1932481	2945243	57.54%	12.495%
9	14.433	1938	1946	1961	rBV	480250	771098	15.06%	3.271%
10	15.933	2194	2201	2220	rBV	1625063	2480569	48.46%	10.524%
11	17.198	2409	2416	2428	rBV	649101	963684	18.83%	4.089%
12	19.480	2799	2804	2808	rBV	146310	159555	3.12%	0.677%
13	19.774	2848	2854	2862	rBV	4166945	5118725	100.00%	21.717%
14	20.498	2974	2977	2982	rVB	112470	123975	2.42%	0.526%
15	21.086	3074	3077	3085	rBV	86602	110840	2.17%	0.470%
16	21.304	3109	3114	3127	rBV	884410	1194621	23.34%	5.068%
17	21.421	3130	3134	3138	rBV	168159	231404	4.52%	0.982%
18	22.415	3300	3303	3308	rVB	87897	111028	2.17%	0.471%
19	22.968	3394	3397	3403	rVB	109279	152441	2.98%	0.647%
20	23.598	3500	3504	3510	rVB	145213	251217	4.91%	1.066%
21	23.698	3515	3521	3533	rVB2	563862	1189721	23.24%	5.048%
22	24.327	3624	3628	3636	rVB2	128230	244646	4.78%	1.038%

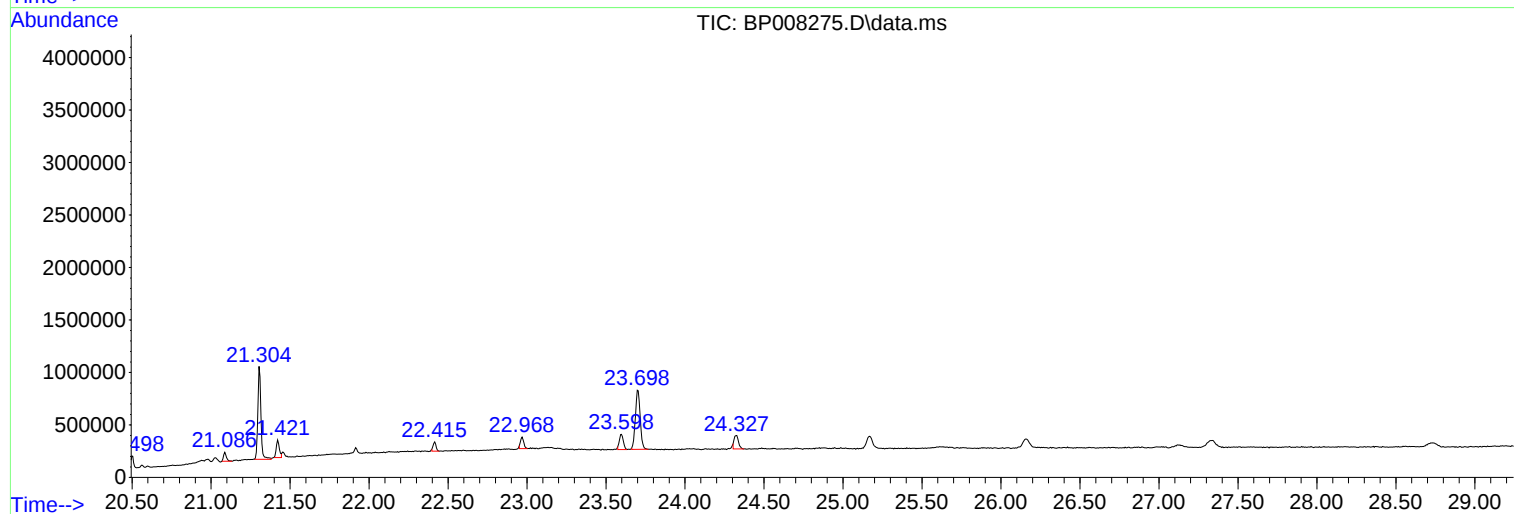
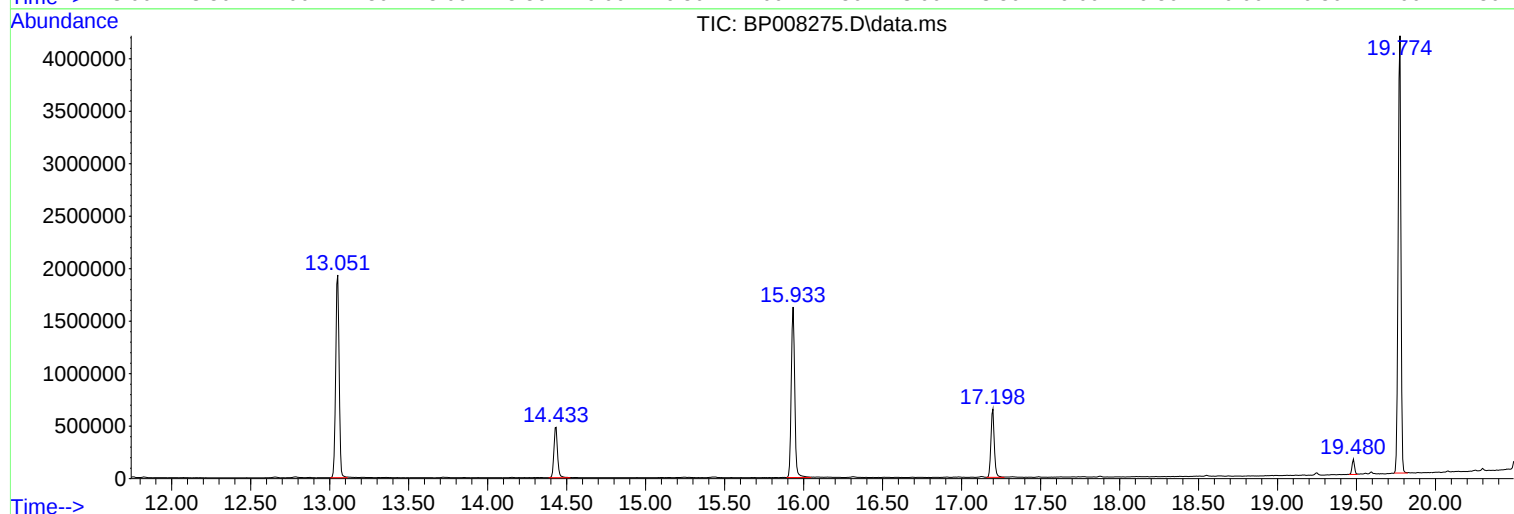
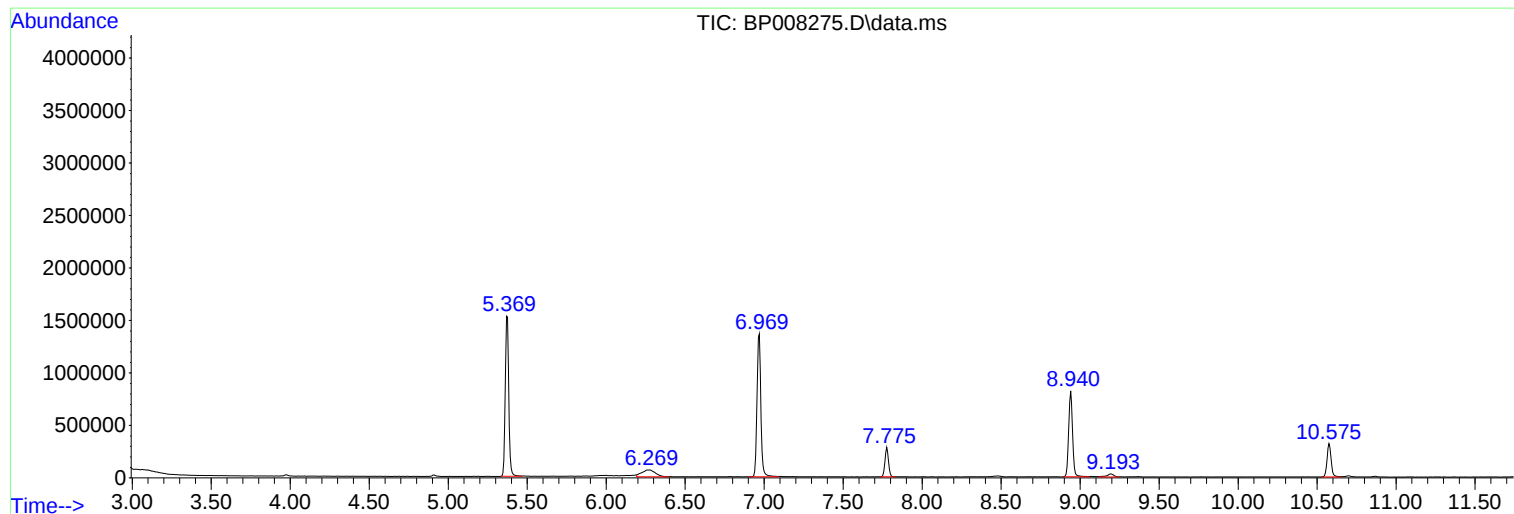
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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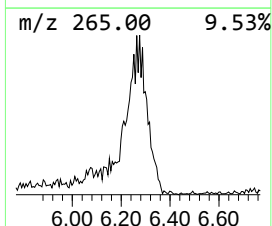
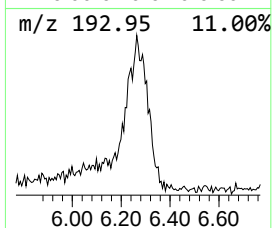
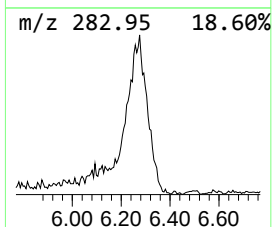
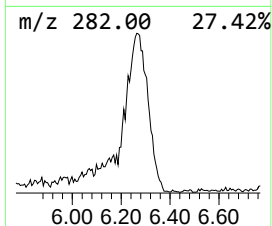
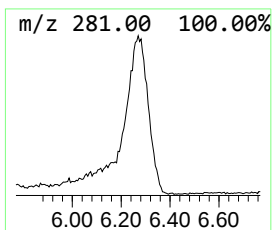
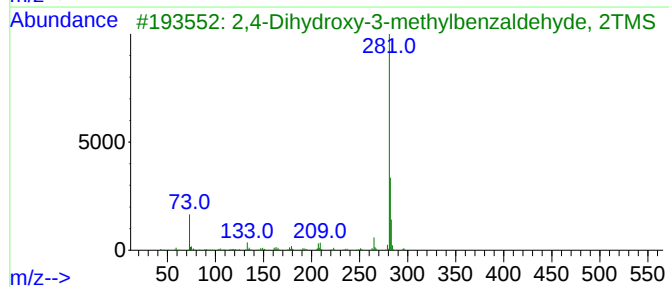
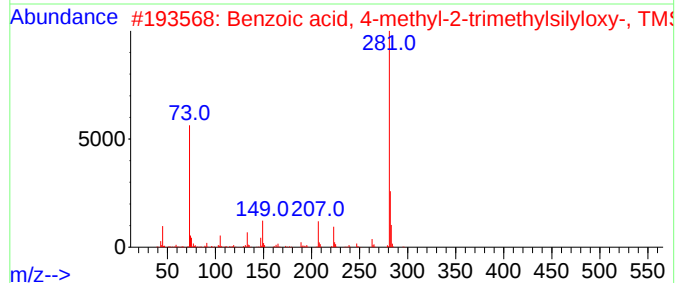
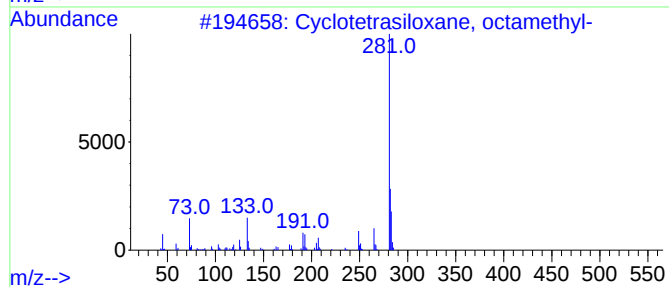
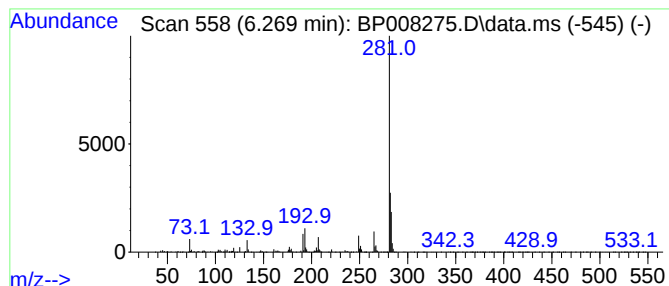
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclotetrasiloxane, octamet... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.269	17.91 ng	386223	1,4-Dichlorobenzene-d4	7.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetrasiloxane, octamethyl-	296	C8H24O4Si4	000556-67-2	90
2			Benzoic acid, 4-methyl-2-trimeth...	296	C14H24O3Si2	1000385-69-8	59
3			2,4-Dihydroxy-3-methylbenzaldehy...	296	C14H24O3Si2	1000514-43-5	50
4			1-(2,4-Dihydroxyphenyl)-2-(4-flu...	406	C20H27F04Si2	1000474-42-3	50
5			trans-4-Dimethylamino-4'-methoxy...	281	C18H19NO2	052119-37-6	50



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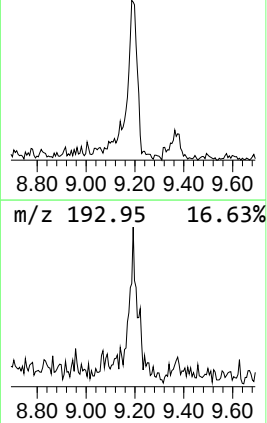
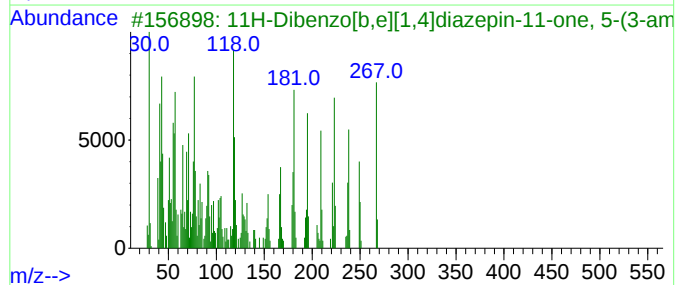
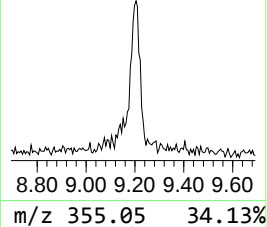
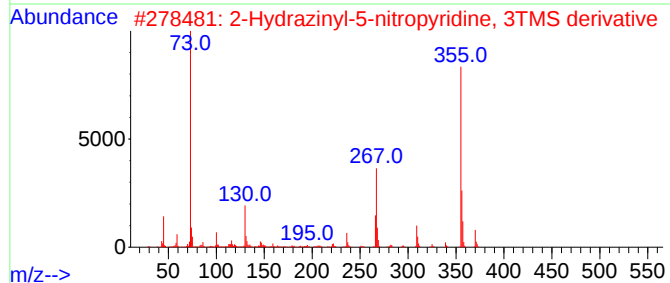
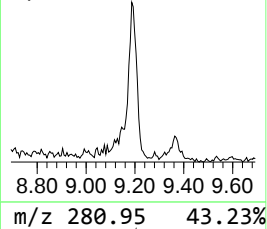
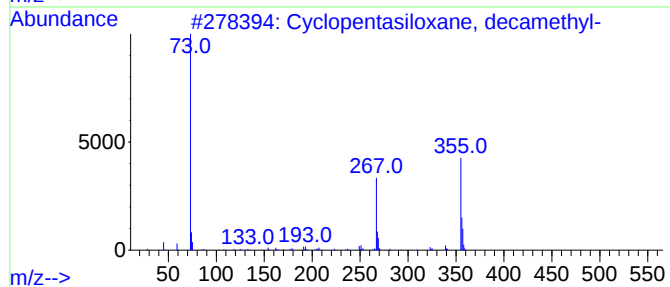
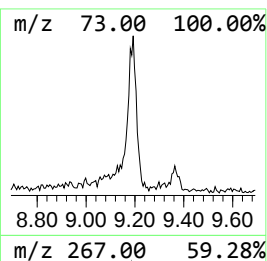
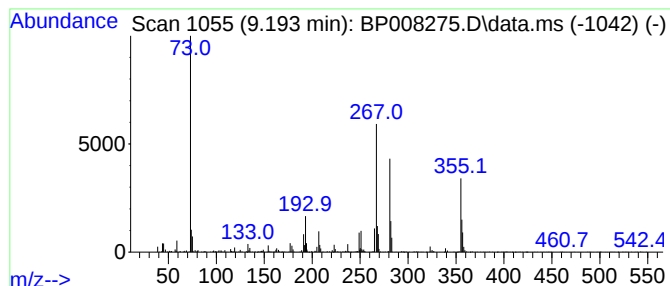
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Peak Number 2 unknown9.193 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.193	2.96 ng	83421	Naphthalene-d8	10.575

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	38
2			2-Hydrazinyl-5-nitropyridine, 3T...	370	C14H30N4O2Si3	1000478-90-5	27
3			11H-Dibenzo[b,e][1,4]diazepin-11...	267	C16H17N3O	013450-73-2	25
4			6-Aminonicotinic acid,N,O di-TMS	282	C12H22N2O2Si2	1000472-37-7	25
5			3,6-Bis(N,N-dimethylamino)-9-met...	267	C17H21N3	119046-55-8	22



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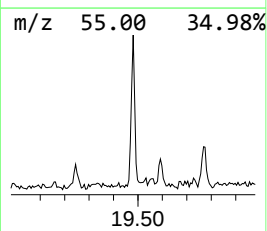
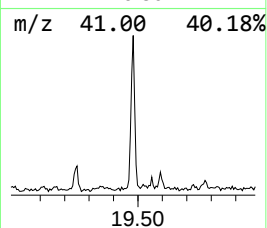
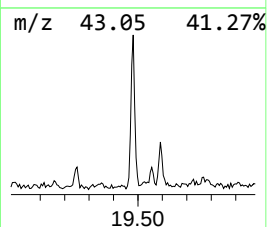
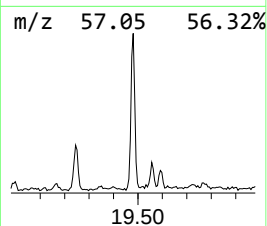
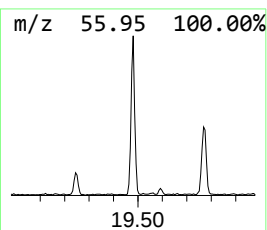
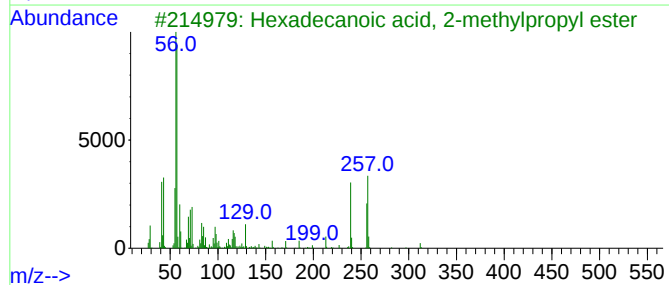
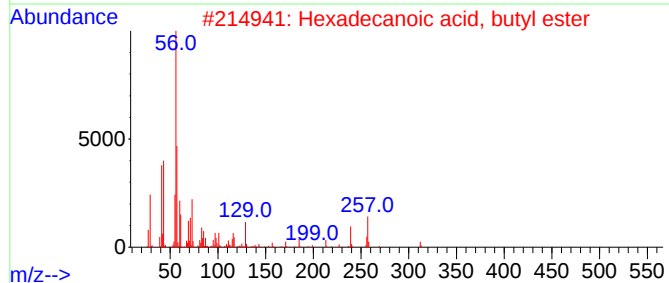
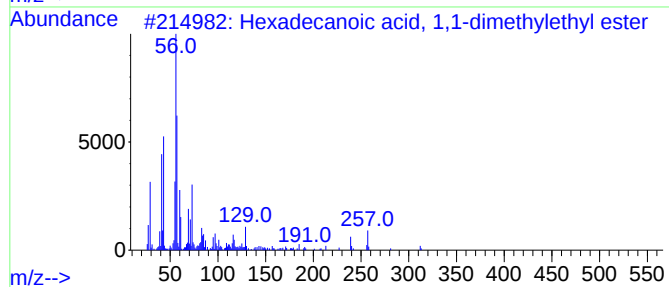
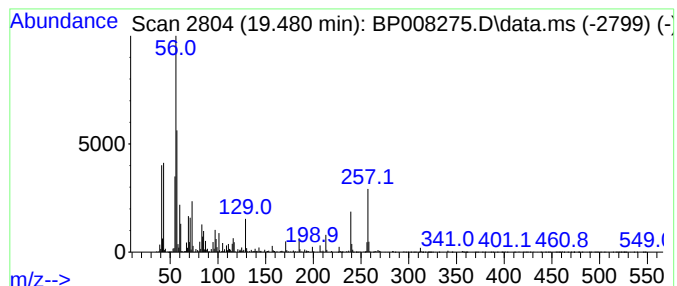
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Peak Number 3 Hexadecanoic acid, 1,1-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.480	2.67 ng	159555	Chrysene-d12	21.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	98
2			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	98
3			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	91
4			2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	47
5			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	35



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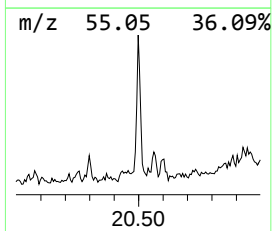
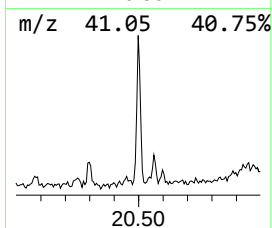
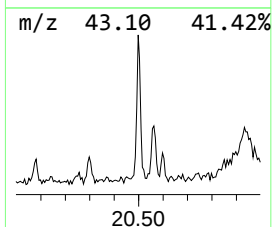
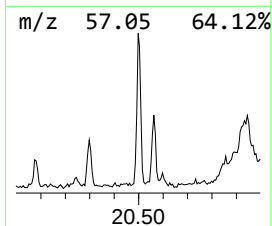
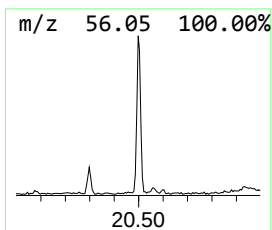
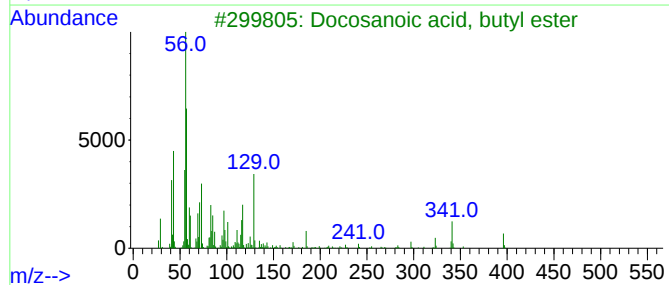
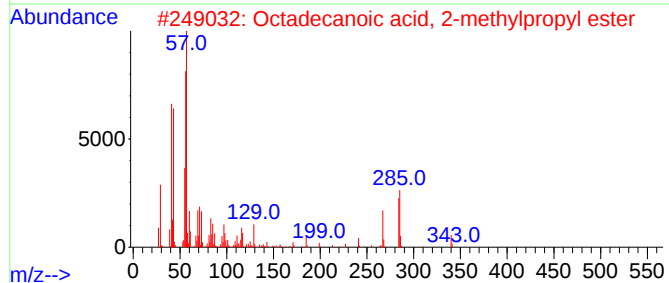
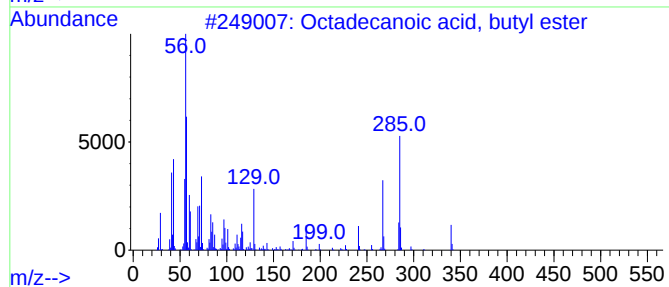
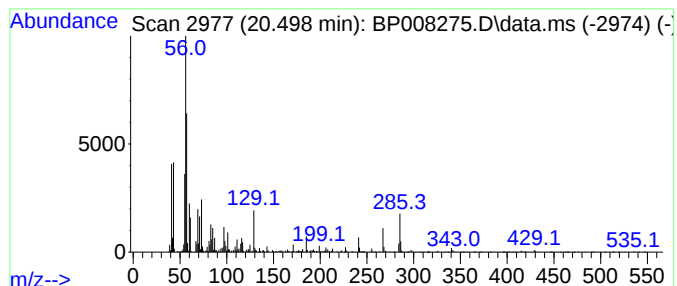
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Peak Number 4 Octadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.498	2.08 ng	123975	Chrysene-d12	21.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	97
2			Octadecanoic acid, 2-methylpropyl...	340	C22H44O2	000646-13-9	43
3			Docosanoic acid, butyl ester	396	C26H52O2	026718-96-7	38
4			1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	37
5			1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27



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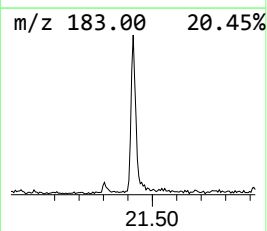
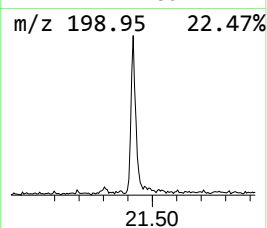
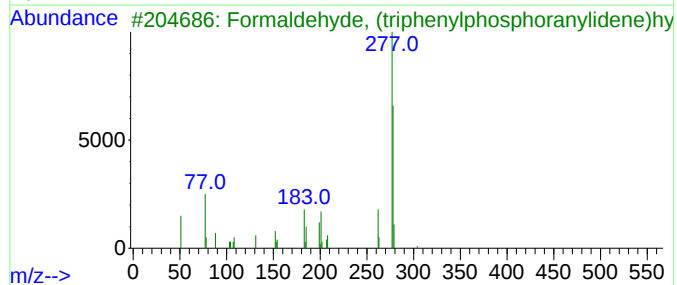
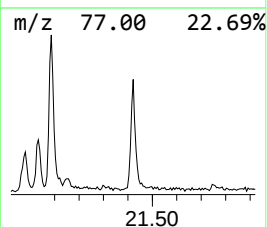
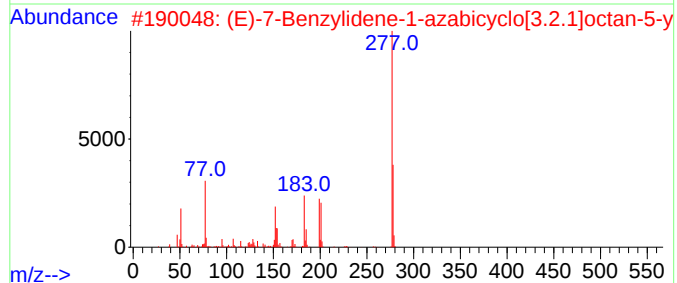
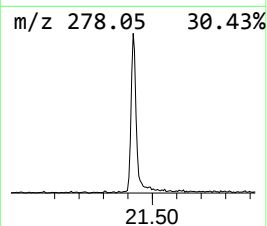
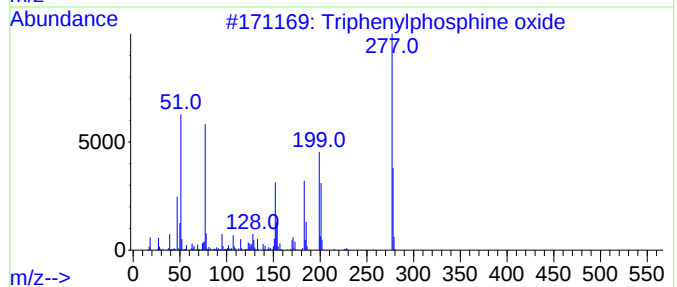
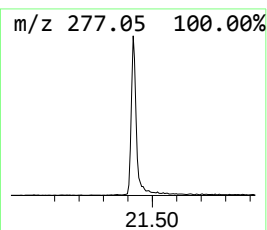
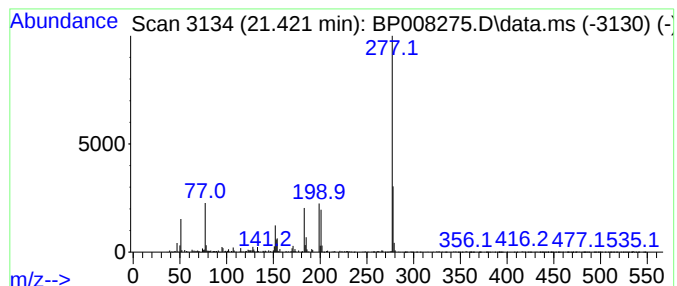
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.421	3.87 ng	231404	Chrysene-d12	21.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	91
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	58
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	50
4			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	43
5			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	38



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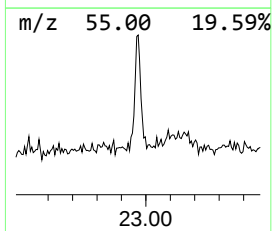
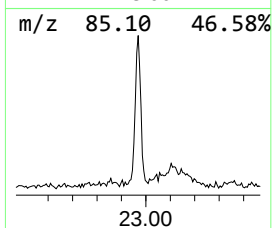
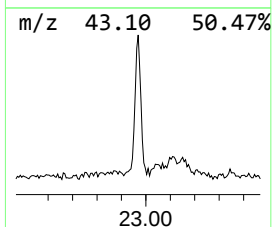
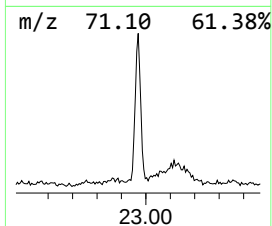
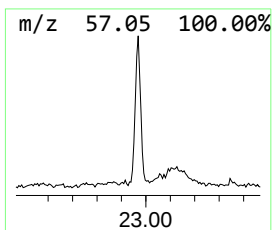
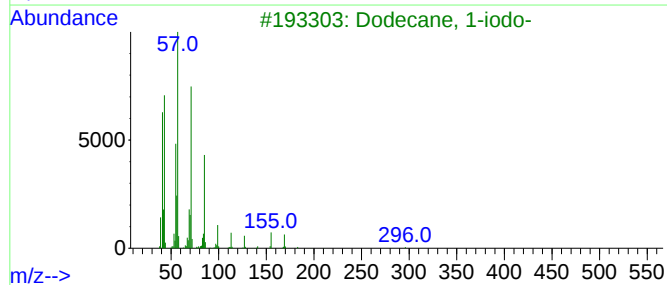
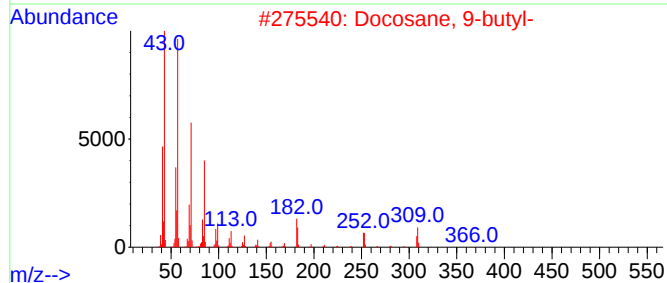
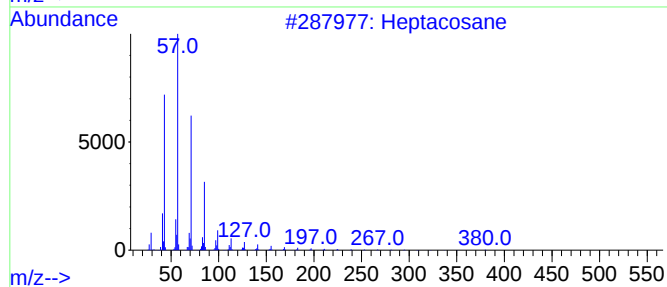
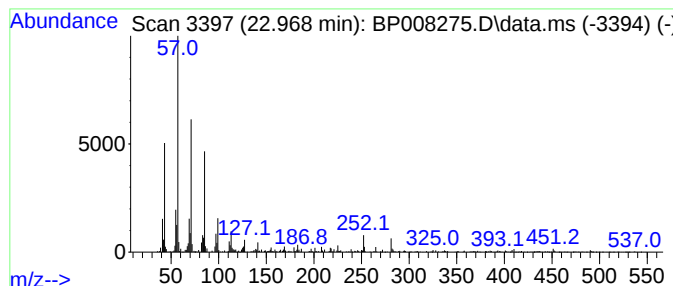
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.968	2.56 ng	152441	Perylene-d12	23.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	98
2			Docosane, 9-butyl-	366	C26H54	055282-14-9	91
3			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	90
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008275.D
Acq On : 08 Dec 2021 11:56
Operator : CG/JU
Sample : PB141209BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB141209BL

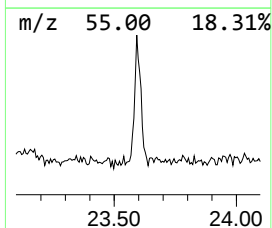
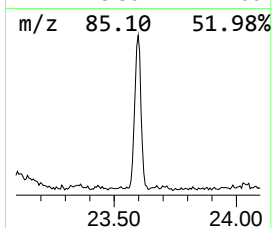
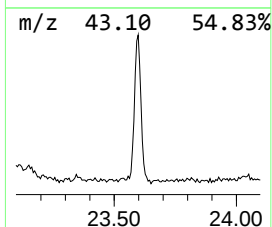
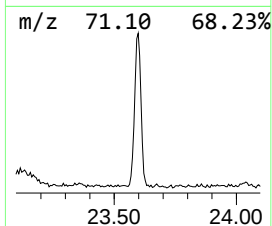
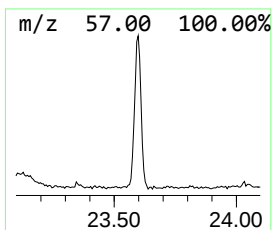
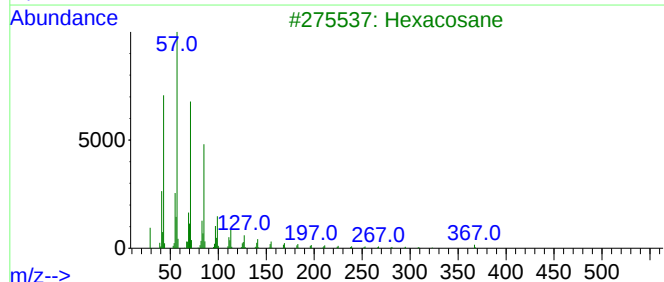
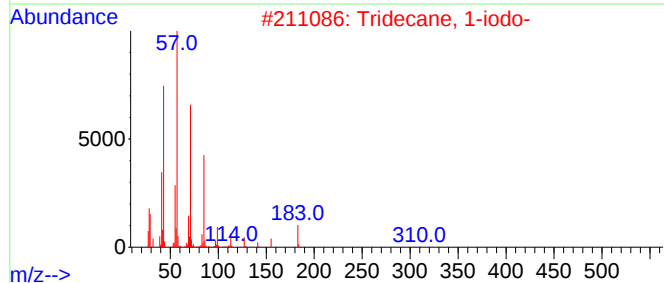
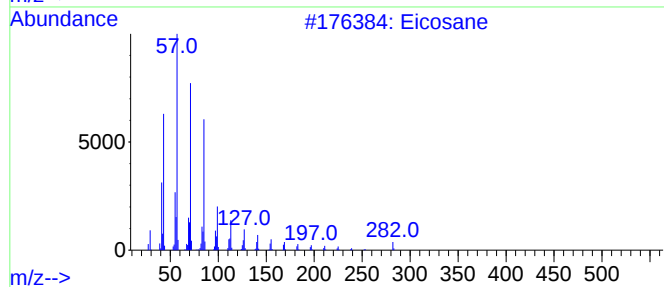
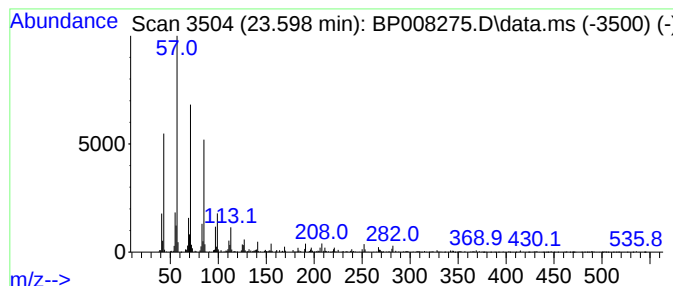
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.598	4.22 ng	251217	Perylene-d12	23.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
3			Hexacosane	366	C26H54	000630-01-3	87
4			Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	87
5			Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008275.D
Acq On : 08 Dec 2021 11:56
Operator : CG/JU
Sample : PB141209BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB141209BL

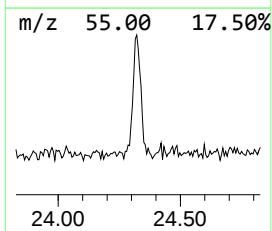
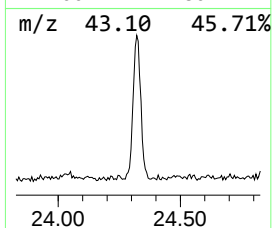
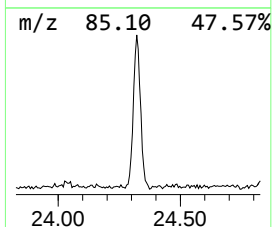
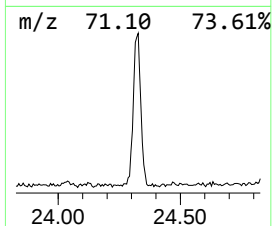
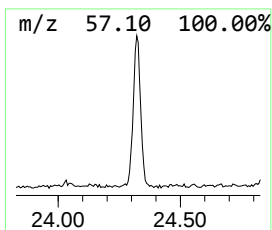
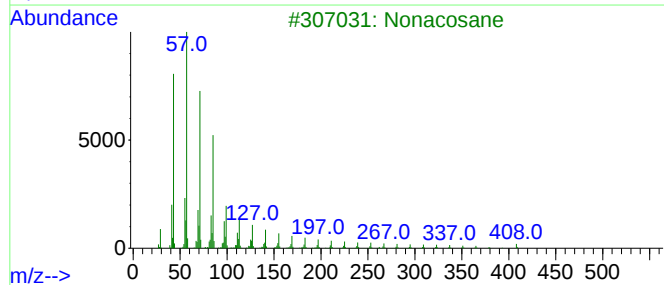
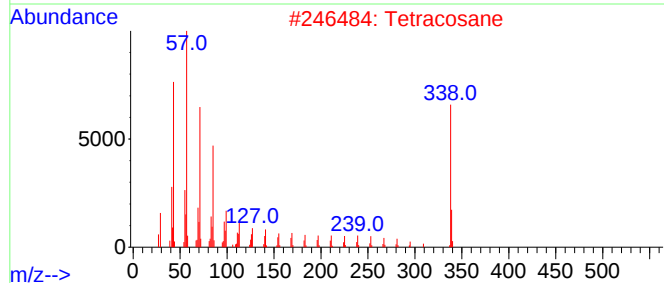
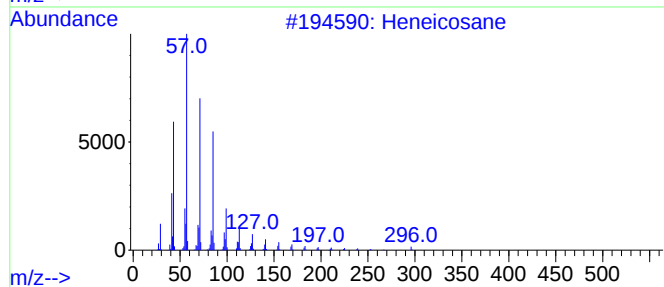
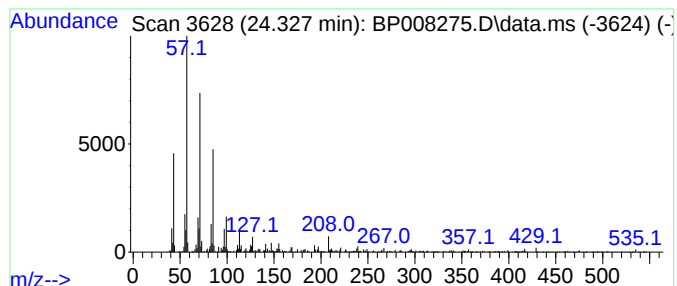
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.327	4.11 ng	244646	Perylene-d12	23.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Tetracosane	338	C24H50	000646-31-1	87
3			Nonacosane	408	C29H60	000630-03-5	87
4			Hexadecane	226	C16H34	000544-76-3	83
5			11-Methyltricosane	338	C24H50	027538-41-6	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008275.D
Acq On : 08 Dec 2021 11:56
Operator : CG/JU
Sample : PB141209BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB141209BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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
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unknown9.193	9.193	3.0	ng	83421	2	10.575	563950	20.0
Hexadecanoic ac...	19.480	2.7	ng	159555	5	21.304	1194620	20.0
Octadecanoic ac...	20.498	2.1	ng	123975	5	21.304	1194620	20.0
Triphenylphosph...	21.421	3.9	ng	231404	5	21.304	1194620	20.0
Heptacosane	22.968	2.6	ng	152441	6	23.698	1189720	20.0
Eicosane	23.598	4.2	ng	251217	6	23.698	1189720	20.0
Heneicosane	24.327	4.1	ng	244646	6	23.698	1189720	20.0