

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051322\
 Data File : BG053552.D
 Acq On : 13 May 2022 21:03
 Operator : CG/JU
 Sample : N2795-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 VNJ-239

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_G\Methods\8270-BG050522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053552.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.651	379	385	398	rVB	427403	691470	37.36%	5.942%
2	7.249	647	657	672	rBV	459333	831378	44.92%	7.144%
3	8.083	793	799	806	rBV	107908	181586	9.81%	1.560%
4	9.247	989	997	1012	rBV	291350	529560	28.61%	4.551%
5	10.891	1269	1277	1285	rBV	145162	270484	14.61%	2.324%
6	13.329	1685	1692	1702	rBV	770777	1254457	67.77%	10.780%
7	14.710	1920	1927	1934	rBV	262028	405198	21.89%	3.482%
8	16.196	2172	2180	2192	rBV	650789	1031919	55.75%	8.867%
9	17.453	2386	2394	2399	rBV	331185	500162	27.02%	4.298%
10	17.494	2399	2401	2410	rVB2	27087	38723	2.09%	0.333%
11	18.334	2539	2544	2549	rBV3	32893	56360	3.04%	0.484%
12	19.245	2695	2699	2703	rVB2	31748	40854	2.21%	0.351%
13	19.503	2737	2743	2750	rBV	63812	91342	4.93%	0.785%
14	19.603	2756	2760	2765	rBV7	14741	25148	1.36%	0.216%
15	19.826	2791	2798	2800	rBV6	16056	34088	1.84%	0.293%
16	19.867	2801	2805	2813	rVB	56842	85053	4.60%	0.731%
17	20.055	2831	2837	2843	rBV	1368657	1850949	100.00%	15.905%
18	20.173	2853	2857	2861	rBV3	12727	18969	1.02%	0.163%
19	20.355	2879	2888	2893	rVB2	69184	97436	5.26%	0.837%
20	21.354	3053	3058	3067	rBV	112278	184693	9.98%	1.587%
21	21.606	3093	3101	3107	rVB	157823	229141	12.38%	1.969%
22	21.735	3114	3123	3128	rBV	328341	600946	32.47%	5.164%
23	22.552	3253	3262	3273	rVB6	45623	165239	8.93%	1.420%
24	22.781	3295	3301	3310	rVB2	34710	76653	4.14%	0.659%
25	22.904	3317	3322	3327	rBV8	13502	25907	1.40%	0.223%
26	23.228	3373	3377	3382	rVB7	15270	28959	1.56%	0.249%
27	23.974	3497	3504	3509	rBV3	21644	63119	3.41%	0.542%
28	24.050	3510	3517	3522	rVV4	41256	101827	5.50%	0.875%
29	24.109	3522	3527	3539	rVB8	30404	85961	4.64%	0.739%
30	24.250	3544	3551	3556	rBV8	10336	25247	1.36%	0.217%
31	24.708	3626	3629	3636	rVB4	12223	24661	1.33%	0.212%
32	24.849	3650	3653	3660	rVB2	11991	22675	1.23%	0.195%
33	25.013	3671	3681	3690	rBV3	195248	565889	30.57%	4.863%
34	26.153	3868	3875	3884	rVB6	29028	88680	4.79%	0.762%
35	26.288	3891	3898	3901	rBV9	23462	57879	3.13%	0.497%
36	28.773	4309	4321	4333	rBV8	46382	201737	10.90%	1.734%

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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_G\Methods\8270-BG050522.M
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37	28.914	4334	4345	4362	rVB5	112008	486375	26.28%	4.179%
38	29.384	4412	4425	4440	rBV3	98052	451716	24.40%	3.882%
39	30.424	4592	4602	4603	rBV10	12975	27688	1.50%	0.238%
40	31.534	4781	4791	4792	rBV2	23782	55992	3.03%	0.481%
41	31.804	4830	4837	4839	rBV8	15392	31239	1.69%	0.268%

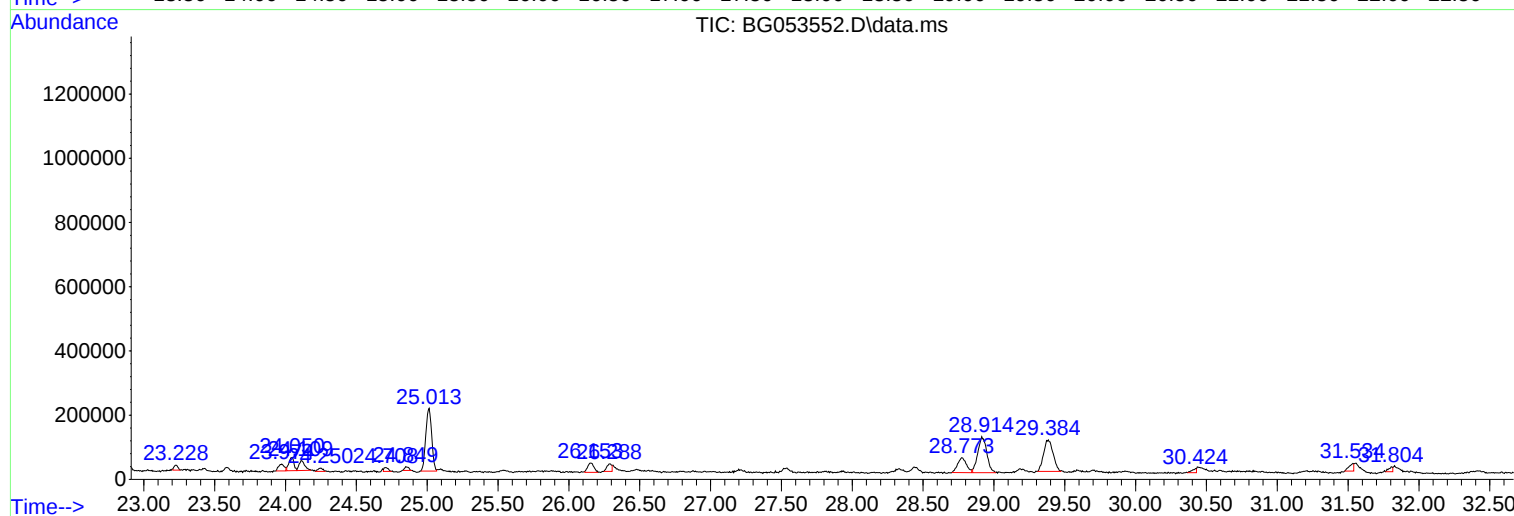
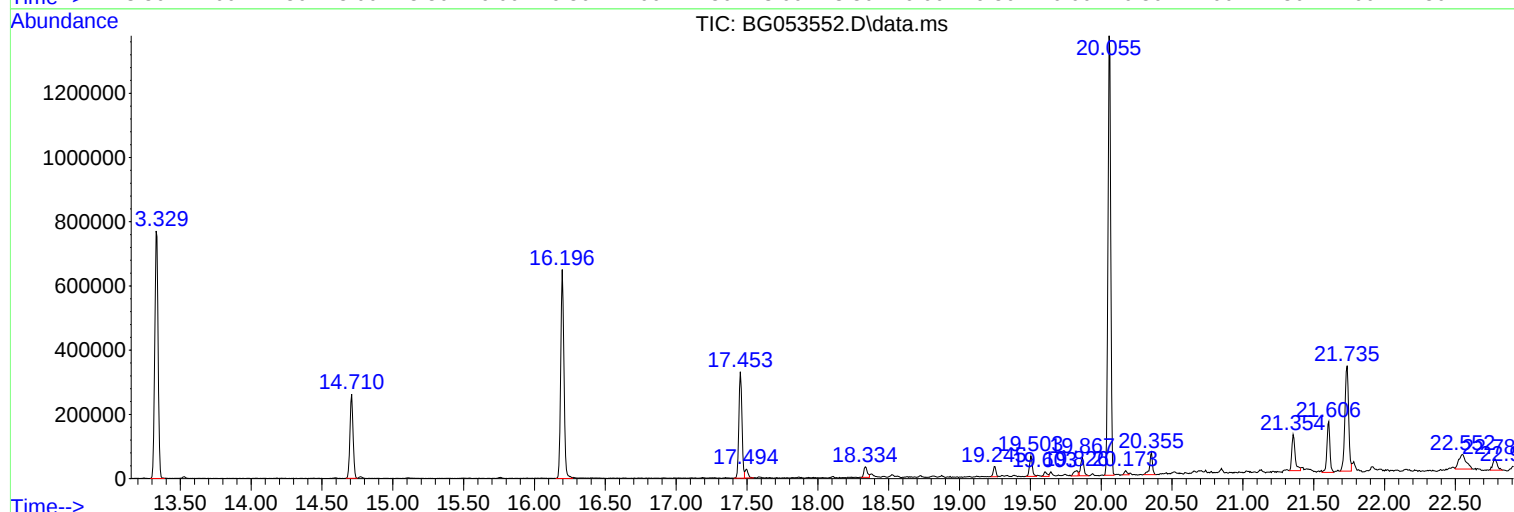
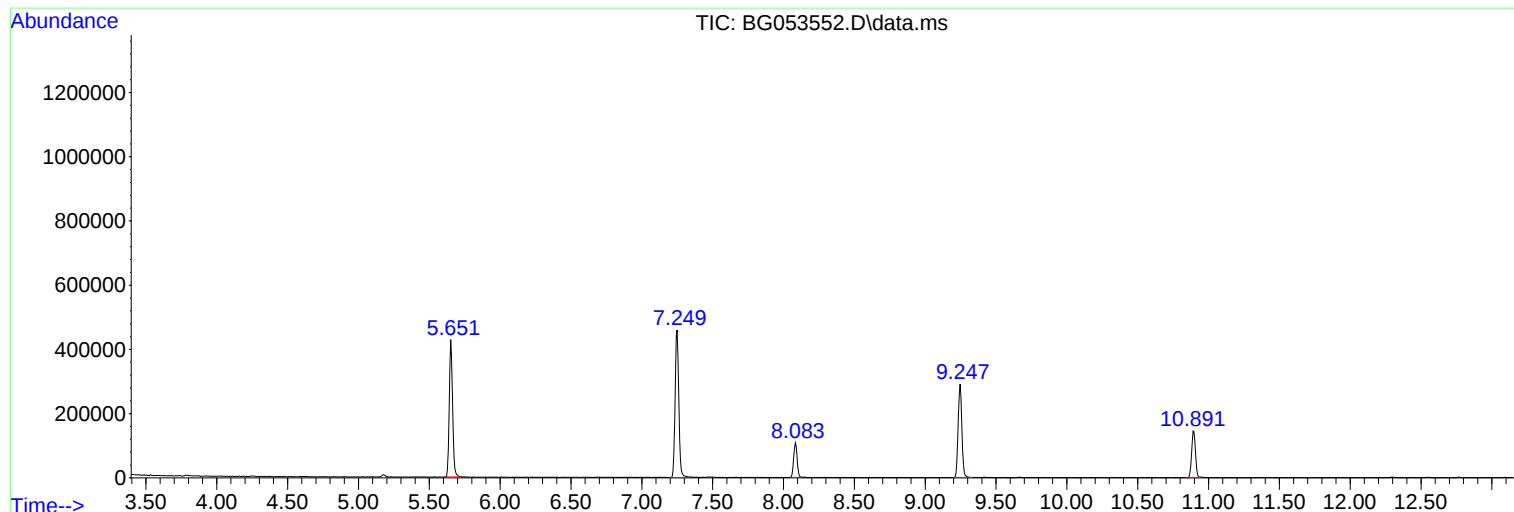
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VNJ-239

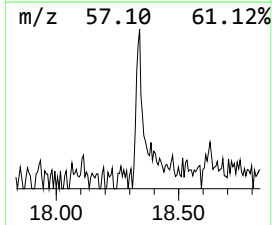
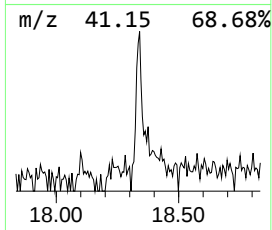
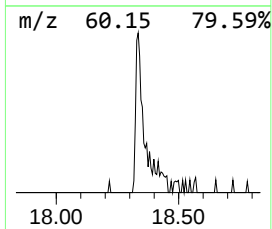
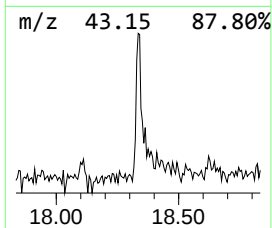
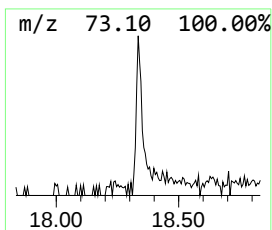
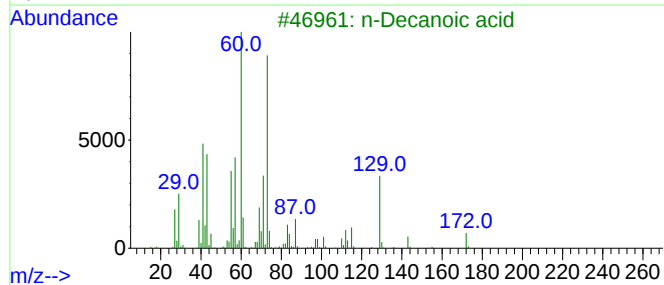
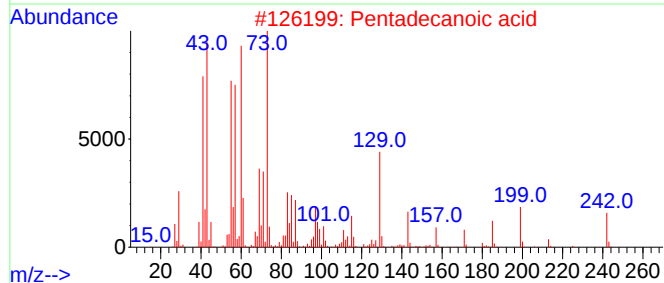
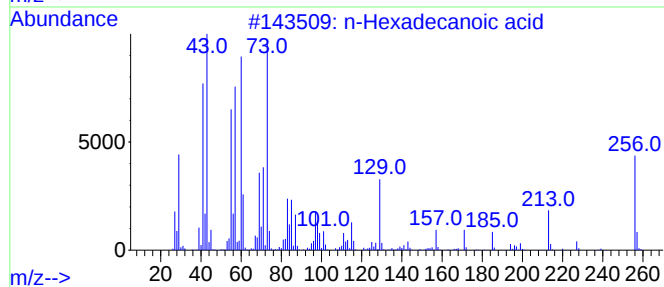
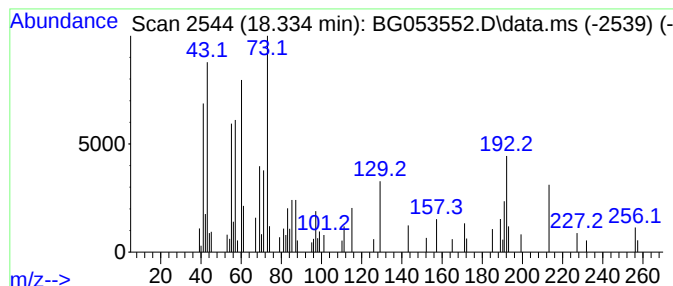
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.334	2.25 ng	56360	Phenanthrene-d10	17.453

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3			n-Decanoic acid	172	C10H20O2	000334-48-5	50
4			Tridecanoic acid	214	C13H26O2	000638-53-9	49
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	47



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Instrument :
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ClientSampleId :
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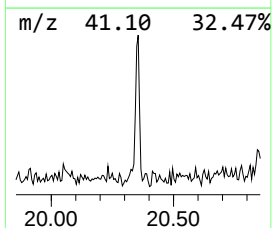
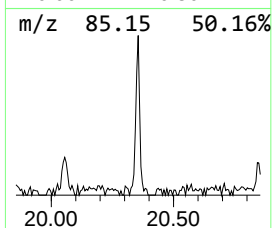
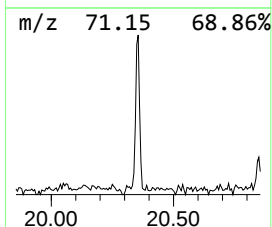
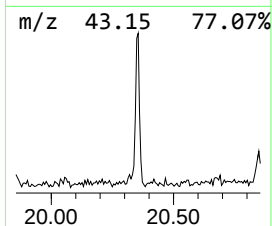
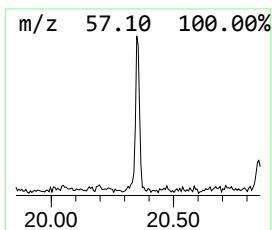
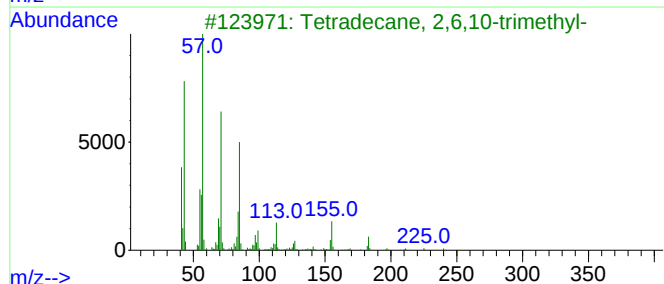
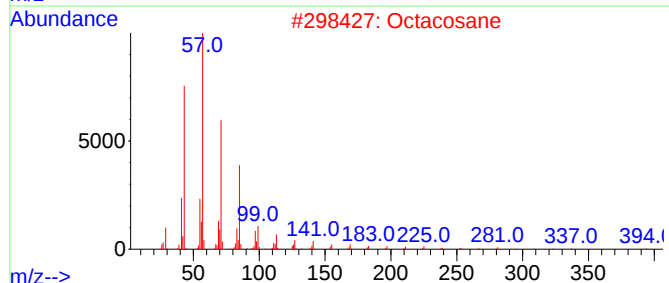
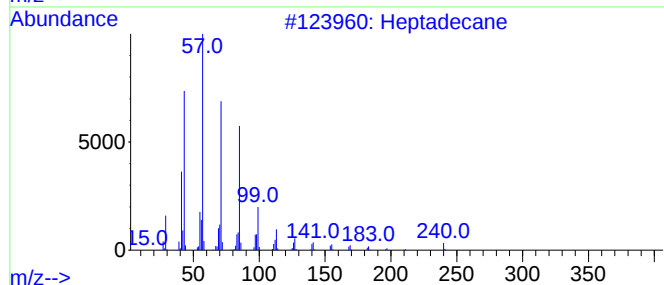
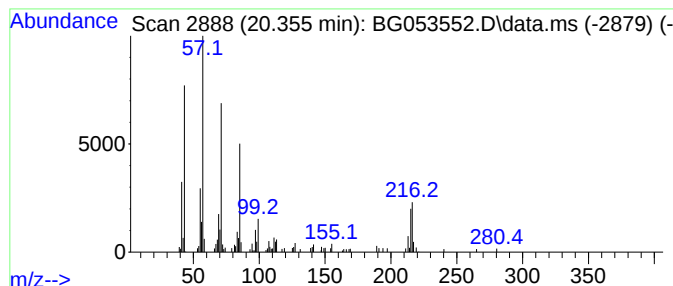
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.355	3.24 ng	97436	Chrysene-d12	21.735

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	95
2		Octacosane	394	C28H58	000630-02-4	70
3		Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	62
4		Tritetracontane	605	C43H88	007098-21-7	58
5		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	58



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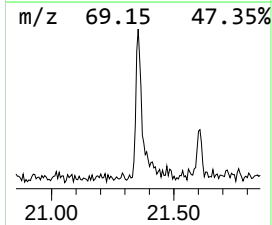
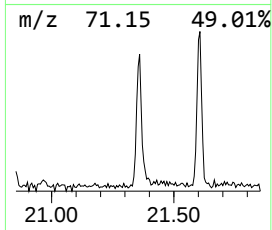
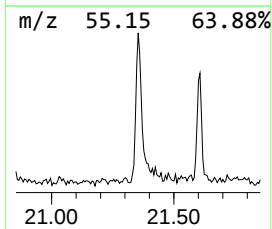
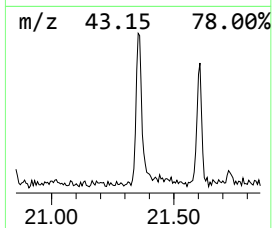
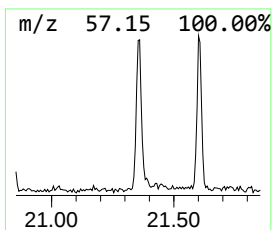
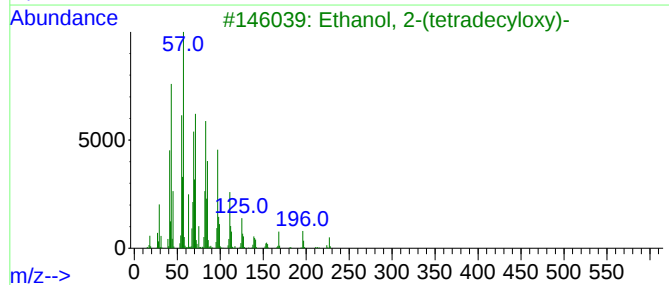
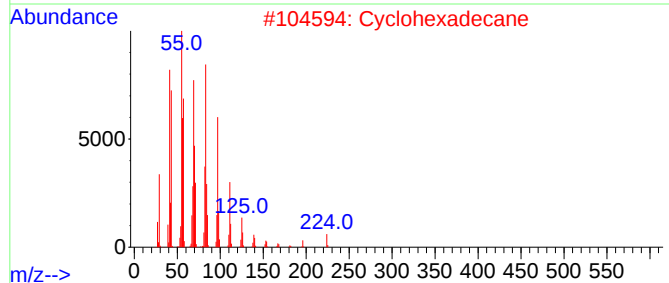
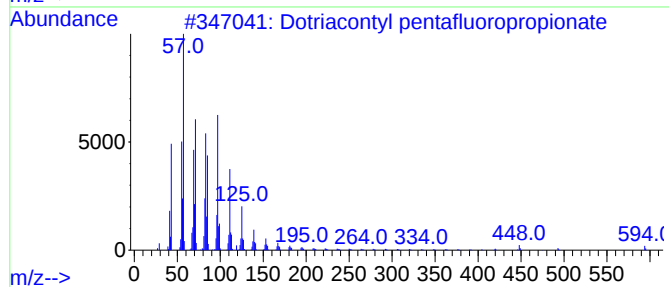
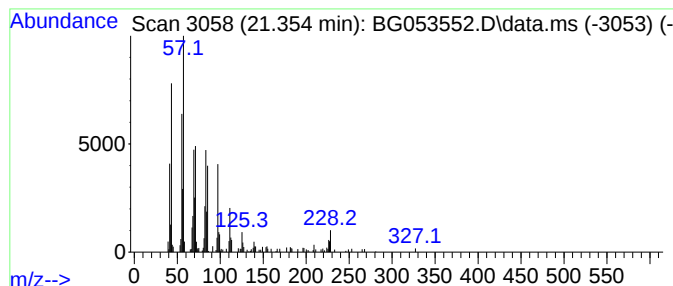
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Dotriacontyl pentafluoropro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.354	6.15 ng	184693	Chrysene-d12	21.735

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1010351-81-4	91
2			Cyclohexadecane	224	C16H32	000295-65-8	87
3			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
4			Hexadecane, 1-(ethenyloxy)-	268	C18H36O	000822-28-6	81
5			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	81



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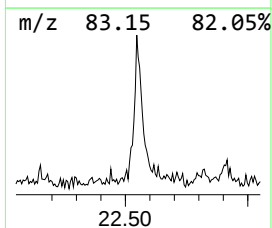
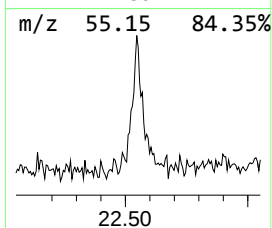
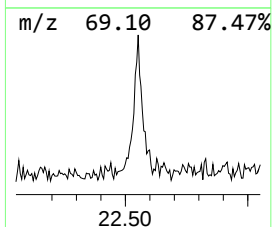
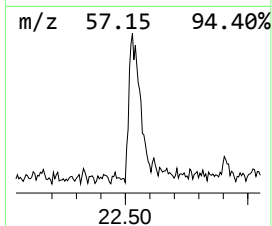
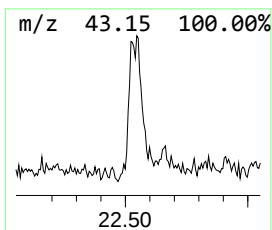
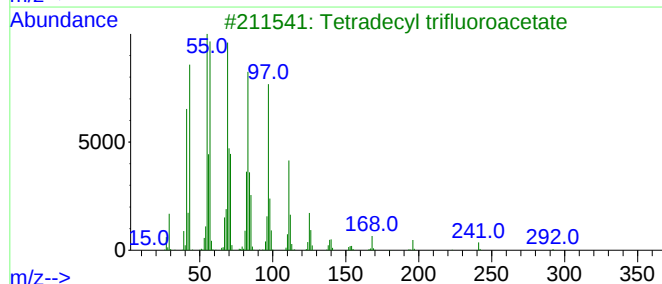
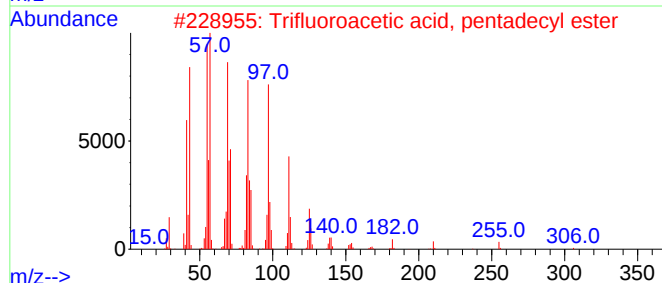
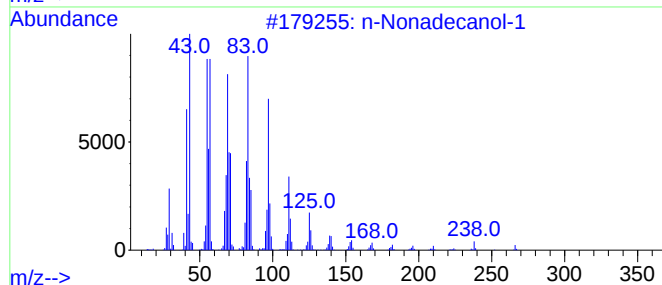
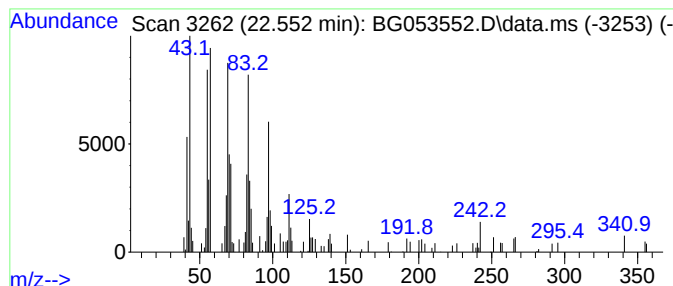
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.552	5.50 ng	165239	Chrysene-d12	21.735

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Nonadecanol-1	284	C19H40O	001454-84-8	93
2		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
3		Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	91
4		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
5		Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	91



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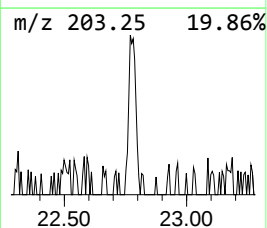
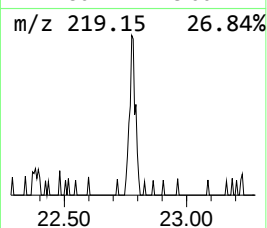
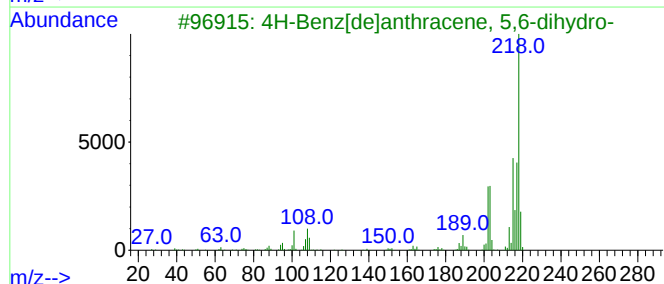
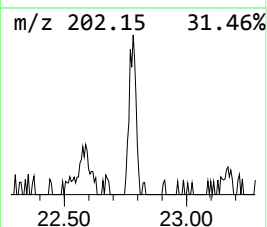
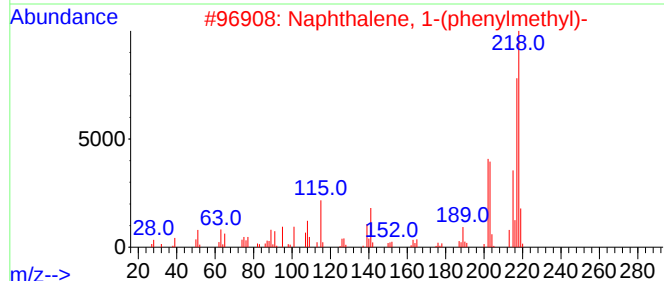
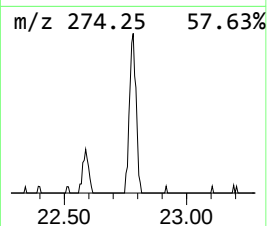
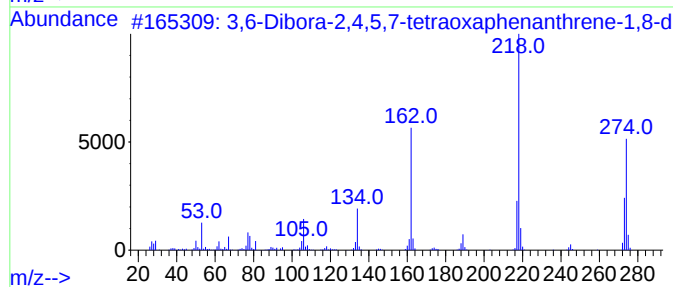
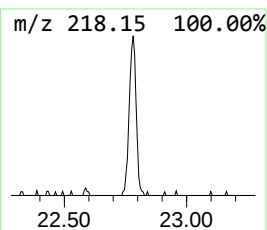
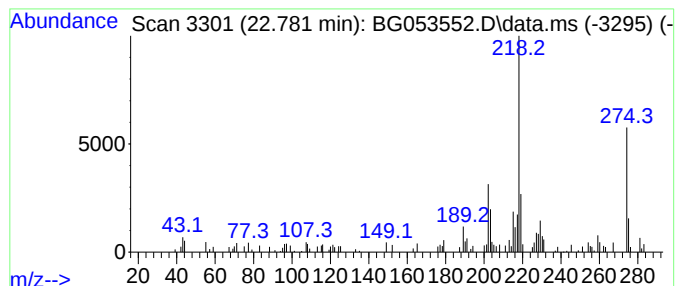
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown22.781 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.781	2.55 ng	76653	Chrysene-d12	21.735

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,6-Dibora-2,4,5,7-tetraoxaphena...	274	C12H12B2O6	1000159-66-2	47
2			Naphthalene, 1-(phenylmethyl)-	218	C17H14	000611-45-0	43
3			4H-Benz[de]anthracene, 5,6-dihydro-	218	C17H14	004389-09-7	43
4			N-Pentafluoropropionyl-L-valine ...	305	C11H16F5NO3	1000139-21-5	38
5			l-Valine, n-pentafluoropropionyl...	459	C22H38F5NO3	1000320-88-8	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051322\
Data File : BG053552.D
Acq On : 13 May 2022 21:03
Operator : CG/JU
Sample : N2795-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-239

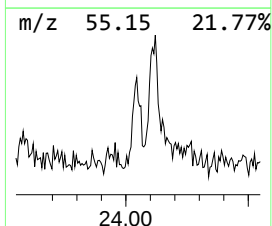
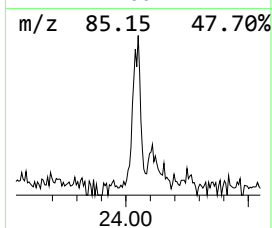
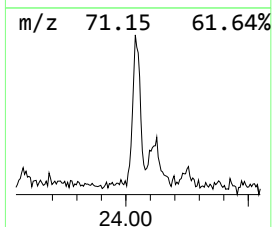
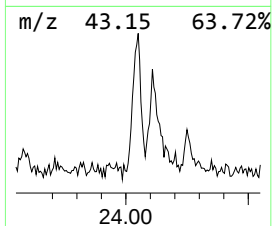
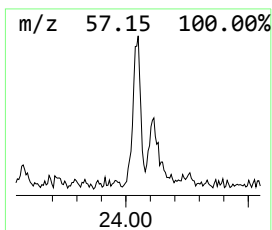
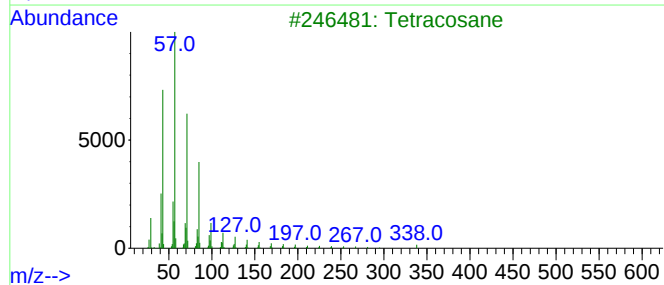
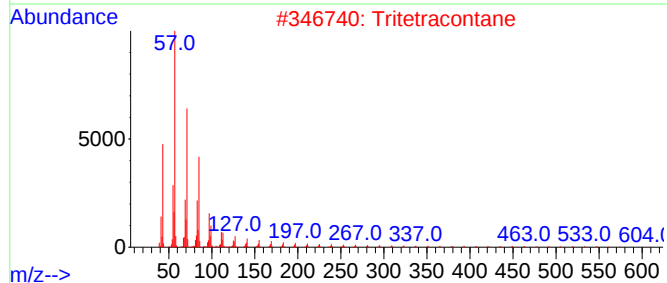
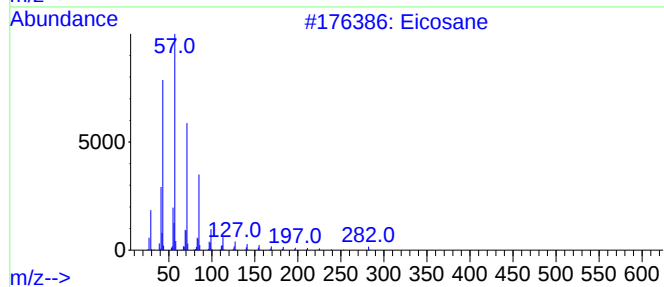
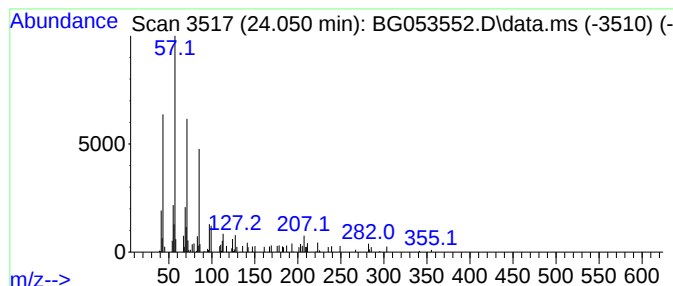
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.050	3.60 ng	101827	Perylene-d12	25.013

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	87
2			Tritetracontane	605	C43H88	007098-21-7	80
3			Tetracosane	338	C24H50	000646-31-1	80
4			Heptadecane	240	C17H36	000629-78-7	80
5			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051322\
Data File : BG053552.D
Acq On : 13 May 2022 21:03
Operator : CG/JU
Sample : N2795-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-239

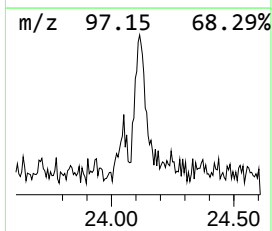
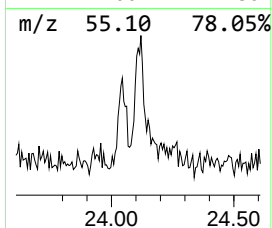
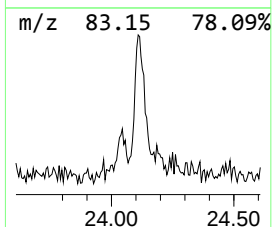
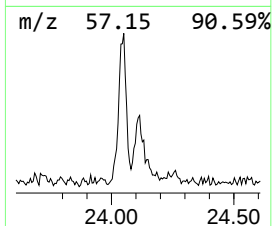
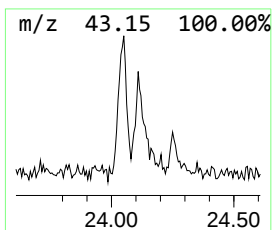
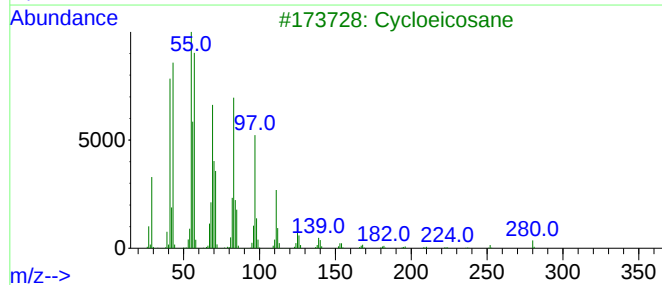
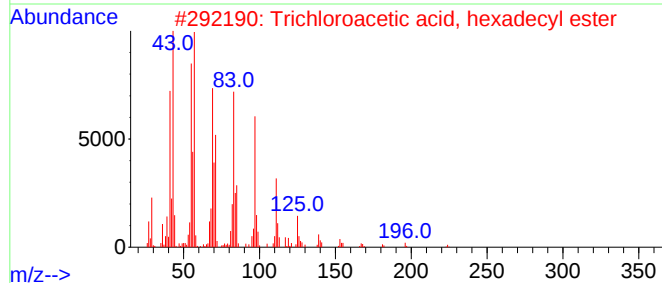
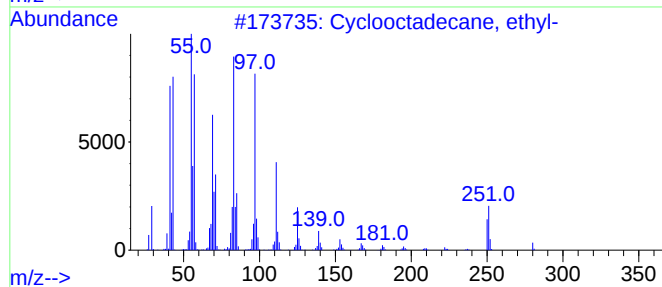
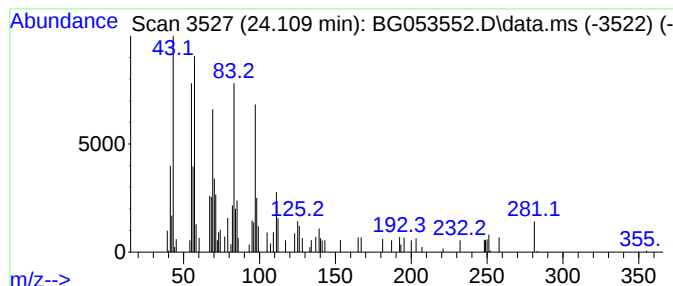
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclooctadecane, ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.109	3.04 ng	85961	Perylene-d12	25.013

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclooctadecane, ethyl-	280	C20H40	1000151-22-5	90
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	83
3			Cycloeicosane	280	C20H40	000296-56-0	83
4			10-Heneicosene (c,t)	294	C21H42	095008-11-0	83
5			1,2-Octadecanediol	286	C18H38O2	020294-76-2	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051322\
Data File : BG053552.D
Acq On : 13 May 2022 21:03
Operator : CG/JU
Sample : N2795-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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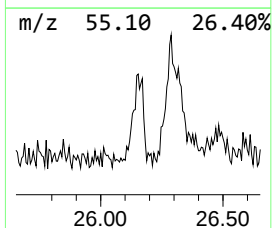
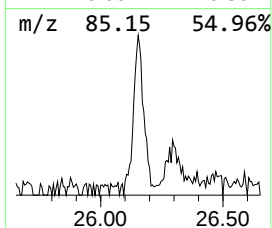
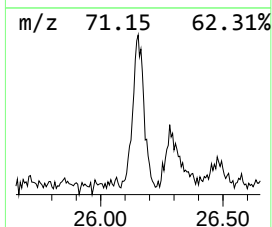
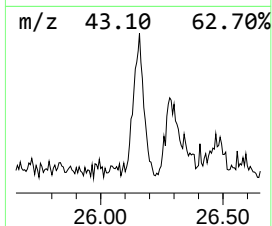
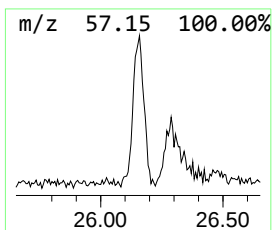
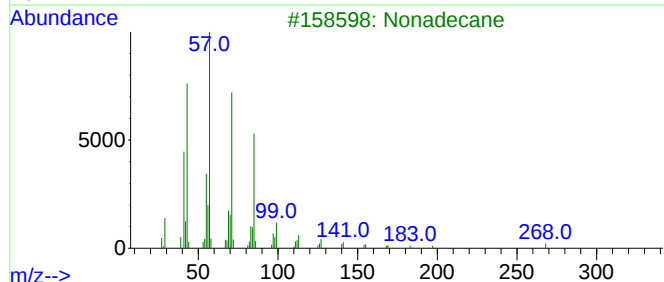
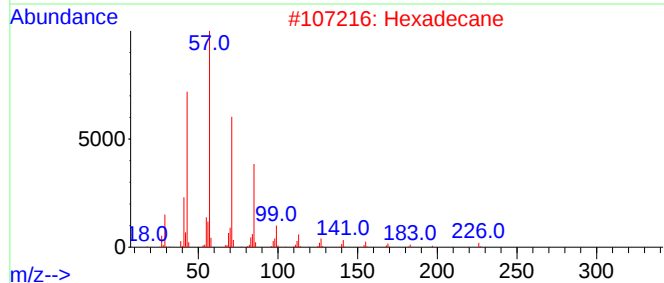
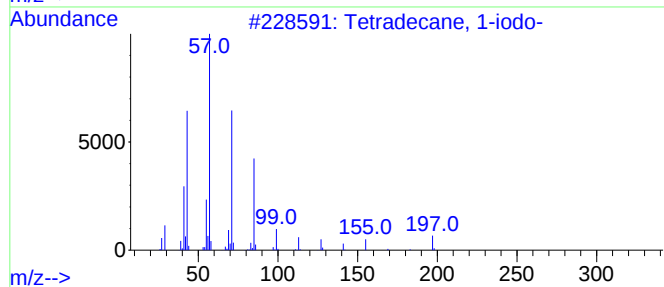
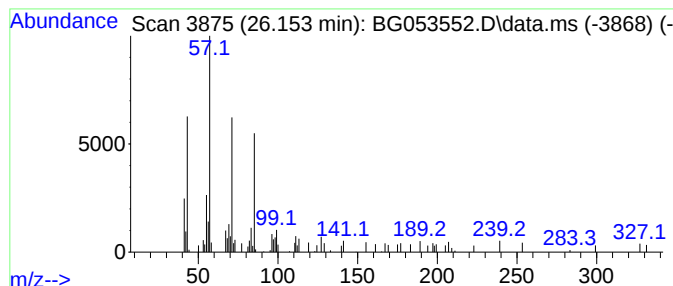
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetradecane, 1-iodo- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.153	3.13 ng	88680	Perylene-d12	25.013

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72
2			Hexadecane	226	C16H34	000544-76-3	72
3			Nonadecane	268	C19H40	000629-92-5	72
4			Tetradecane	198	C14H30	000629-59-4	64
5			Heptadecane	240	C17H36	000629-78-7	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051322\
Data File : BG053552.D
Acq On : 13 May 2022 21:03
Operator : CG/JU
Sample : N2795-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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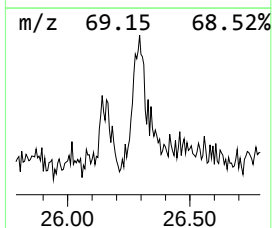
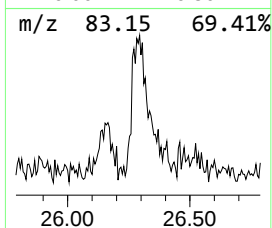
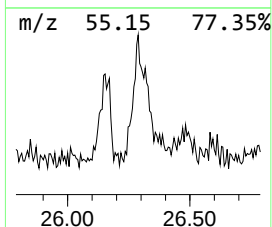
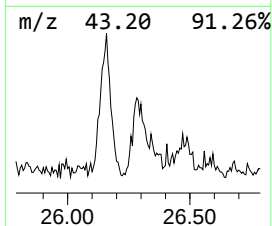
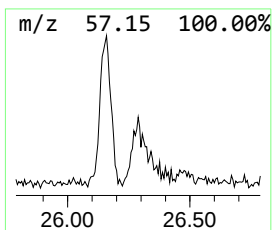
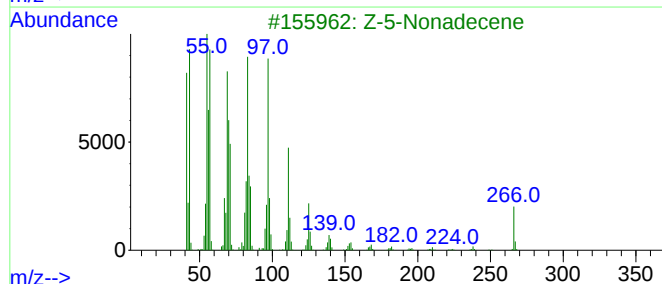
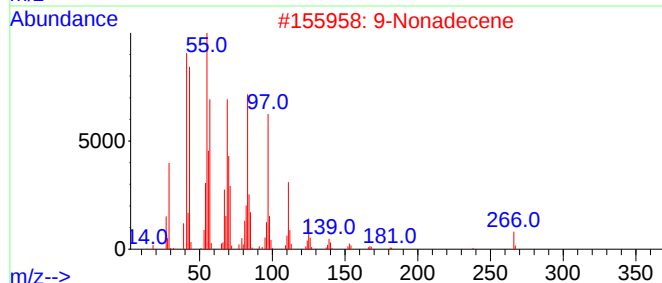
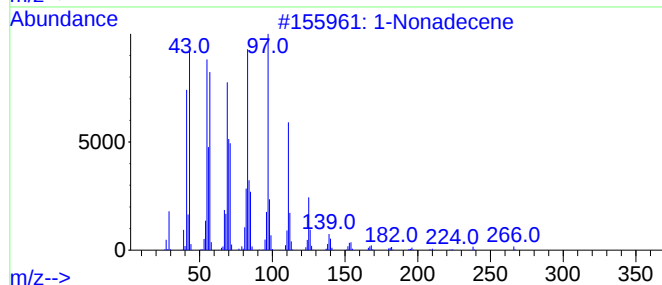
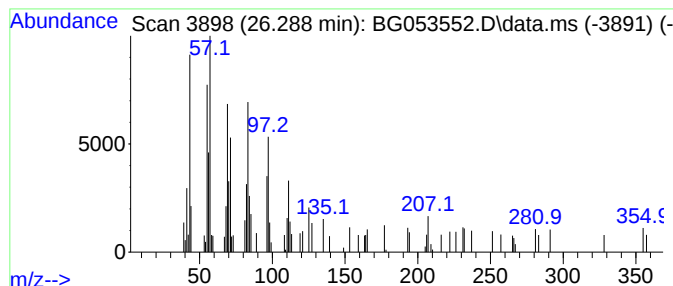
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Nonadecene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.288	2.05 ng	57879	Perylene-d12	25.013

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene			266	C19H38	018435-45-5	74
2	9-Nonadecene			266	C19H38	031035-07-1	55
3	Z-5-Nonadecene			266	C19H38	1000131-11-8	55
4	Cyclopentadecane			210	C15H30	000295-48-7	53
5	1-Octadecanol			270	C18H38O	000112-92-5	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051322\
Data File : BG053552.D
Acq On : 13 May 2022 21:03
Operator : CG/JU
Sample : N2795-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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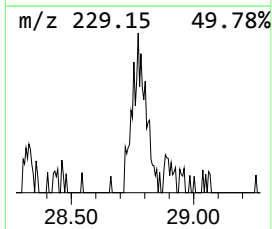
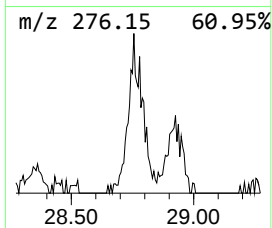
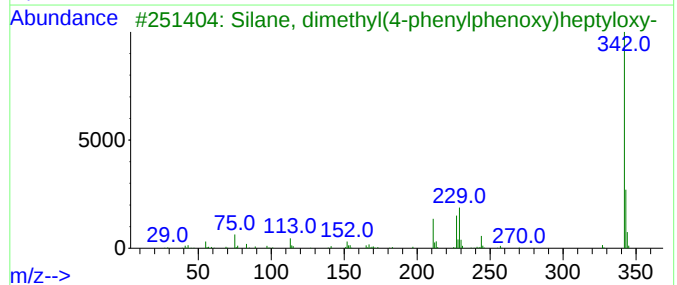
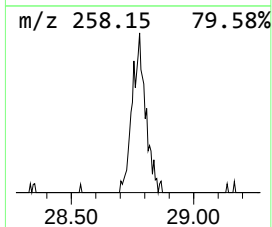
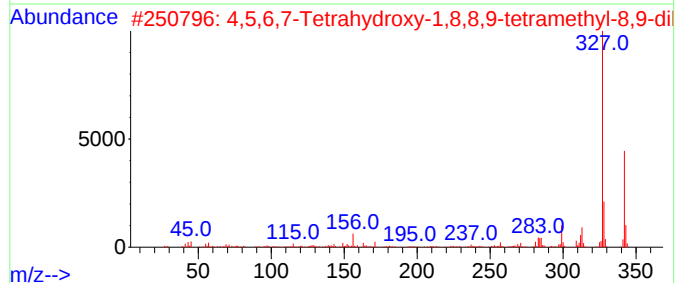
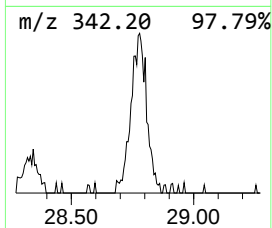
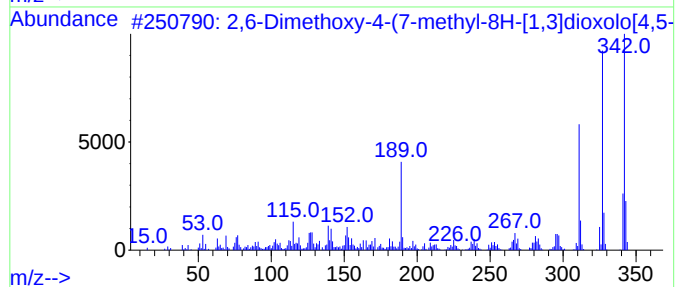
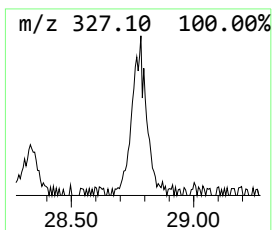
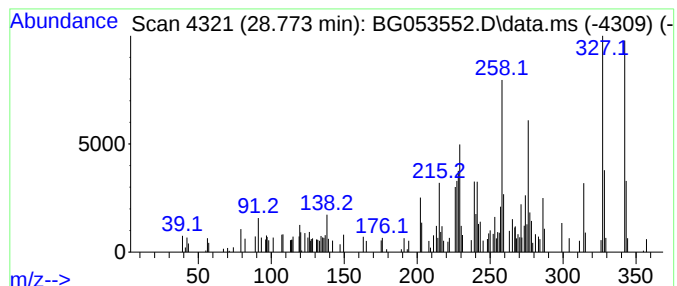
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown28.773 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.773	7.13 ng	201737	Perylene-d12	25.013

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,6-Dimethoxy-4-(7-methyl-8H-[1,...	342	C19H18O6	1000442-99-6	41
2		4,5,6,7-Tetrahydroxy-1,8,8,9-tet...	342	C19H18O6	002582-86-7	38
3		Silane, dimethyl(4-phenylphenoxy...	342	C21H30O2Si	1000347-49-0	35
4		Benzenamine, 4-(9H-carbazol-9-yl)-	258	C18H14N2	052708-37-9	25
5		2',5'-Dimethyl-p-terphenyl	258	C20H18	020260-22-4	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051322\
Data File : BG053552.D
Acq On : 13 May 2022 21:03
Operator : CG/JU
Sample : N2795-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

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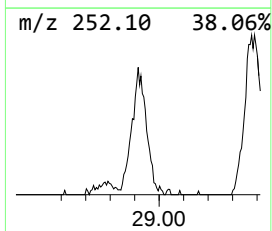
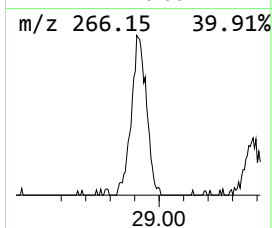
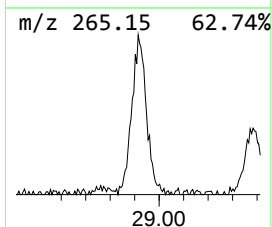
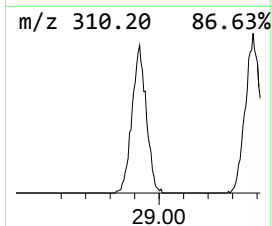
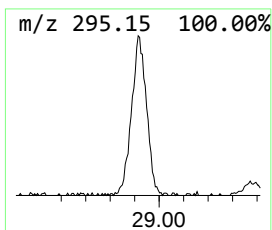
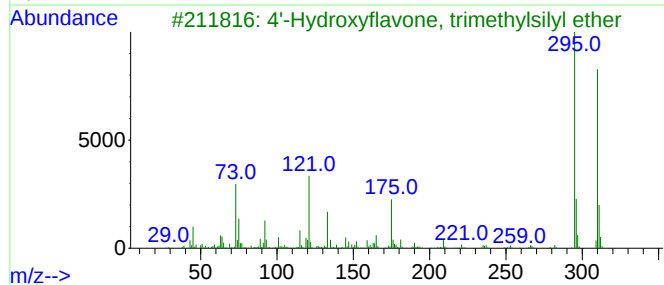
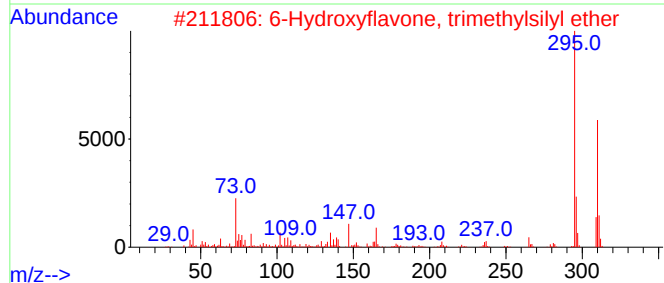
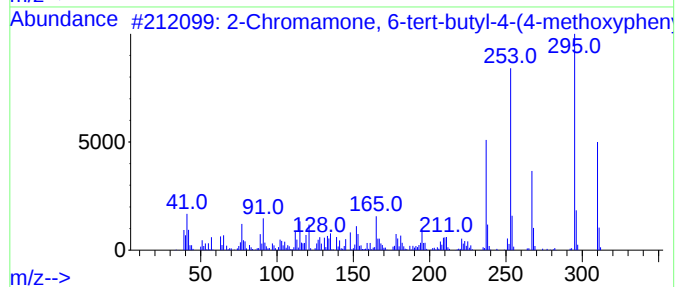
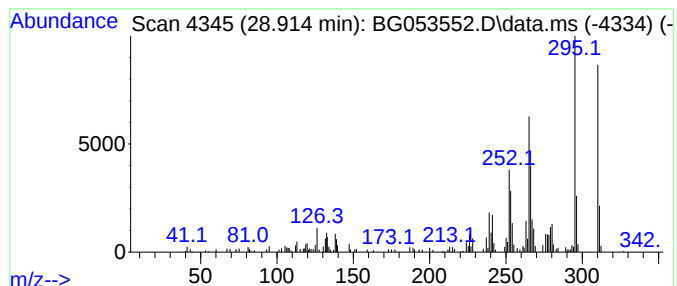
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown28.914 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.914	17.19 ng	486375	Perylene-d12	25.013

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chromamone, 6-tert-butyl-4-(4...	310	C20H22O3	1000276-68-1	49		
2	6-Hydroxyflavone, trimethylsilyl...	310	C18H18O3Si	1000454-60-4	49		
3	4'-Hydroxyflavone, trimethylsily...	310	C18H18O3Si	1010448-92-9	43		
4	2-Amino-5-isopropyl-6,7-dimethox...	295	C17H17N3O2	1000240-33-8	41		
5	2-Hydroxy-3-methylantraquinone,...	310	C18H18O3Si	091701-15-4	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051322\
Data File : BG053552.D
Acq On : 13 May 2022 21:03
Operator : CG/JU
Sample : N2795-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

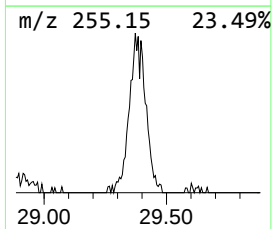
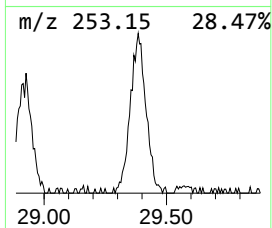
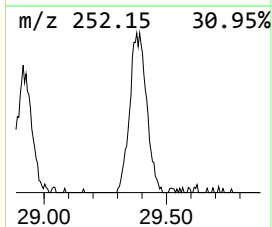
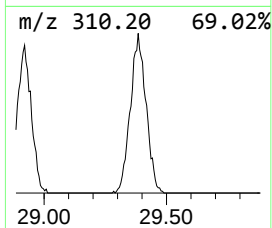
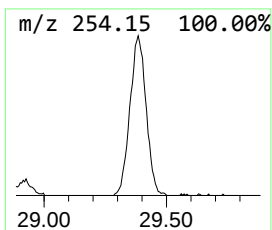
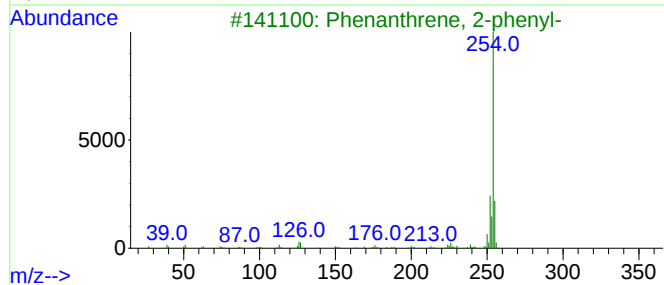
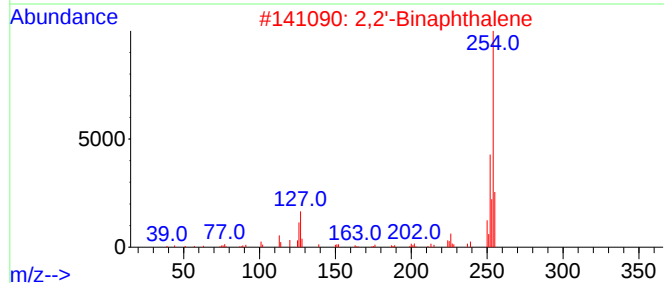
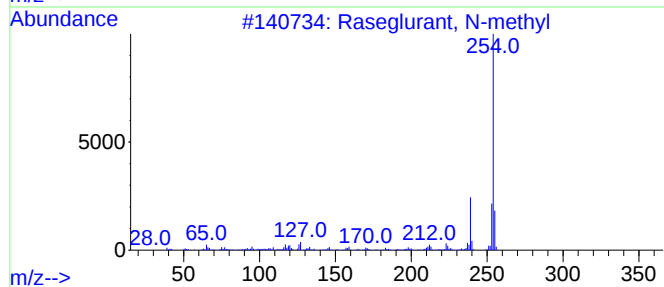
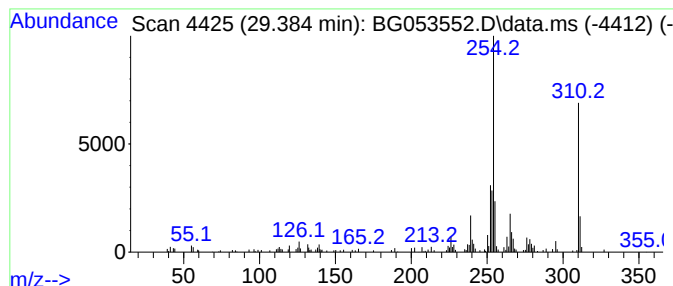
Instrument :
BNA_G
ClientSampleId :
VNJ-239

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown29.384 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
29.384	15.96 ng	451716	Perylene-d12	25.013	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Raseglurant, N-methyl	254	C16H15FN2	1000498-91-9	49
2	2,2'-Binaphthalene	254	C20H14	000612-78-2	46
3	Phenanthrene, 2-phenyl-	254	C20H14	004325-77-3	45
4	Pyrrolo[3,2-g]quinoline, 9-metho...	254	C16H18N2O	199918-71-3	43
5	1,1'-Binaphthalene	254	C20H14	000604-53-5	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051322\
Data File : BG053552.D
Acq On : 13 May 2022 21:03
Operator : CG/JU
Sample : N2795-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-239

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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 ...	18.334	2.3	ng	56360	4	17.453	500162	20.0
Heptadecane	20.355	3.2	ng	97436	5	21.735	600946	20.0
Dotriacontyl pe...	21.354	6.2	ng	184693	5	21.735	600946	20.0
n-Nonadecanol-1	22.552	5.5	ng	165239	5	21.735	600946	20.0
unknown22.781	22.781	2.5	ng	76653	5	21.735	600946	20.0
Eicosane	24.050	3.6	ng	101827	6	25.013	565889	20.0
Cyclooctadecane...	24.109	3.0	ng	85961	6	25.013	565889	20.0
Tetradecane, 1-...	26.153	3.1	ng	88680	6	25.013	565889	20.0
1-Nonadecene	26.288	2.0	ng	57879	6	25.013	565889	20.0
unknown28.773	28.773	7.1	ng	201737	6	25.013	565889	20.0
unknown28.914	28.914	17.2	ng	486375	6	25.013	565889	20.0
unknown29.384	29.384	16.0	ng	451716	6	25.013	565889	20.0