

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
 Data File : BF128305.D
 Acq On : 17 May 2022 22:07
 Operator : CG\JU
 Sample : N2856-01
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HR-02-051322

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-BF050922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128305.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.469	20	31	40	rBV3	11982	26590	1.00%	0.180%
2	4.534	379	382	389	rVB	32341	38307	1.45%	0.259%
3	5.298	509	512	520	rBV	97362	107187	4.05%	0.724%
4	5.498	542	546	554	rBV	1015571	978223	36.95%	6.608%
5	6.434	701	705	711	rBV	27168	29423	1.11%	0.199%
6	6.510	715	718	731	rBV	952186	1044727	39.46%	7.058%
7	6.745	755	758	765	rVB2	26996	28702	1.08%	0.194%
8	6.875	776	780	784	rBV	705137	541245	20.44%	3.656%
9	7.034	801	807	822	rBV	2136862	2647342	100.00%	17.884%
10	7.440	872	876	879	rBV	811442	640897	24.21%	4.330%
11	7.510	885	888	891	rBV	58573	46093	1.74%	0.311%
12	7.892	950	953	960	rBV3	28729	41734	1.58%	0.282%
13	8.081	979	985	991	rBV6	11533	27040	1.02%	0.183%
14	8.157	995	998	1001	rVV	793907	650867	24.59%	4.397%
15	8.187	1001	1003	1009	rVB2	27953	33525	1.27%	0.226%
16	8.439	1044	1046	1051	rVB	36230	34831	1.32%	0.235%
17	8.498	1053	1056	1059	rBV	34780	33282	1.26%	0.225%
18	9.234	1177	1181	1184	rBV	1361573	1038474	39.23%	7.015%
19	9.498	1223	1226	1229	rBV	62342	51690	1.95%	0.349%
20	9.916	1294	1297	1301	rVB	767263	610792	23.07%	4.126%
21	10.116	1328	1331	1336	rVB3	39664	37294	1.41%	0.252%
22	10.333	1366	1368	1370	rVB	37004	26656	1.01%	0.180%
23	10.710	1428	1432	1436	rBV	630967	524699	19.82%	3.545%
24	10.822	1446	1451	1459	rBV6	56157	117954	4.46%	0.797%
25	10.880	1459	1461	1463	rBV	33212	33379	1.26%	0.225%
26	11.033	1480	1487	1489	rBV4	27285	58307	2.20%	0.394%
27	11.063	1489	1492	1496	rVV3	112082	97368	3.68%	0.658%
28	11.098	1496	1498	1501	rBV	35732	30579	1.16%	0.207%
29	11.257	1522	1525	1528	rBV2	99370	103601	3.91%	0.700%
30	11.286	1528	1530	1533	rVB	54279	46456	1.75%	0.314%
31	11.410	1547	1551	1554	rBV	670405	569334	21.51%	3.846%
32	11.433	1554	1555	1561	rVB	100210	66110	2.50%	0.447%
33	11.639	1587	1590	1595	rBV3	29339	44975	1.70%	0.304%
34	11.686	1595	1598	1601	rVV	73116	64917	2.45%	0.439%
35	11.786	1612	1615	1618	rBV	146024	113479	4.29%	0.767%
36	11.939	1636	1641	1644	rBV	1067399	1097072	41.44%	7.411%

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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_F\Methods\8270-BF050922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.092	1665	1667	1670	rVB	91521	65630	2.48%	0.443%
38	12.145	1674	1676	1682	rBV	65033	81867	3.09%	0.553%
39	12.480	1731	1733	1738	rBV3	84624	108235	4.09%	0.731%
40	12.516	1738	1739	1743	rVB	78821	60031	2.27%	0.406%
41	12.580	1748	1750	1755	rBV	117247	110975	4.19%	0.750%
42	12.627	1755	1758	1763	rBV	228151	347038	13.11%	2.344%
43	12.722	1771	1774	1780	rBV	546588	564232	21.31%	3.812%
44	12.857	1795	1797	1800	rBV	192290	160619	6.07%	1.085%
45	12.998	1817	1821	1824	rBV	982637	860557	32.51%	5.813%
46	14.063	1999	2002	2005	rBV	461497	419910	15.86%	2.837%
47	15.563	2254	2257	2261	rVB2	266910	340640	12.87%	2.301%

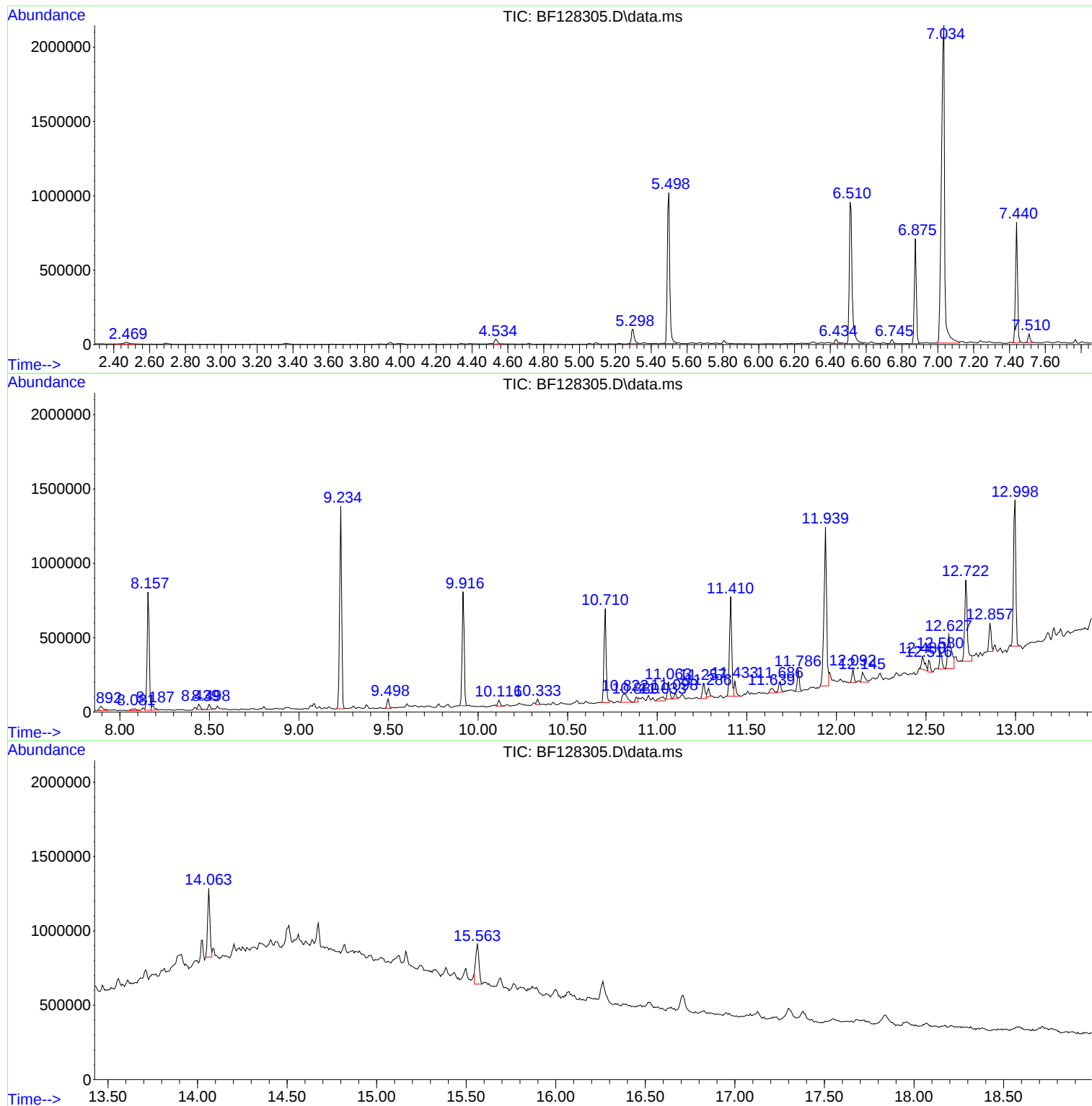
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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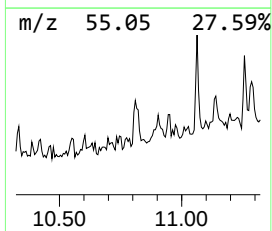
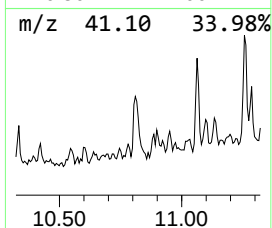
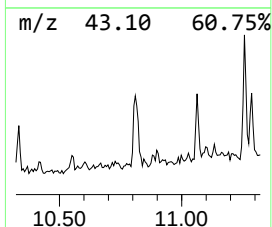
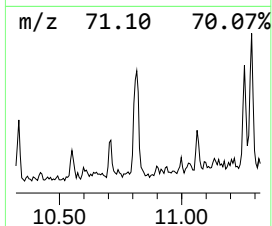
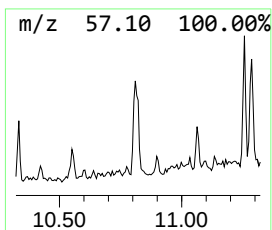
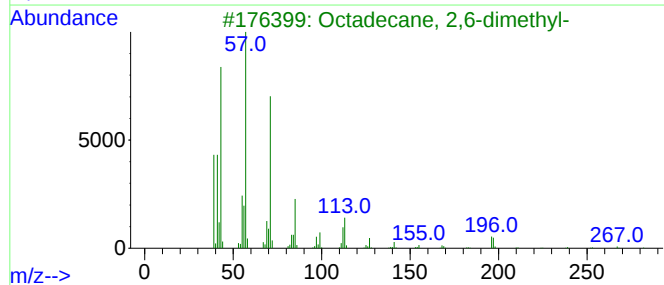
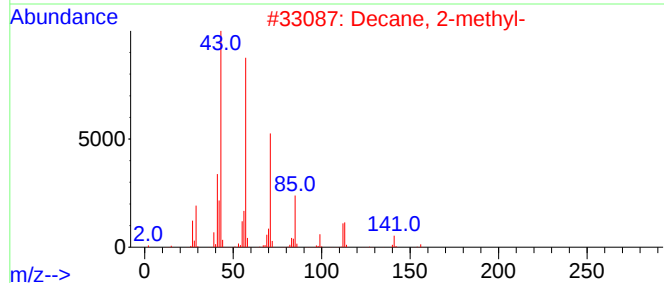
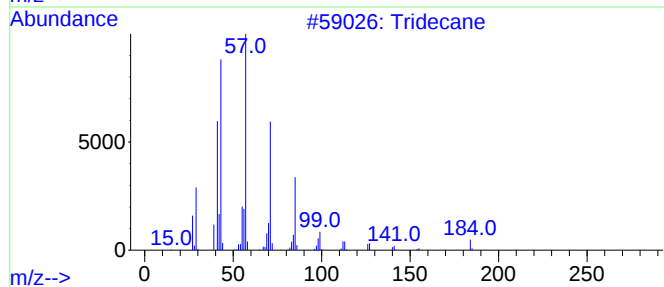
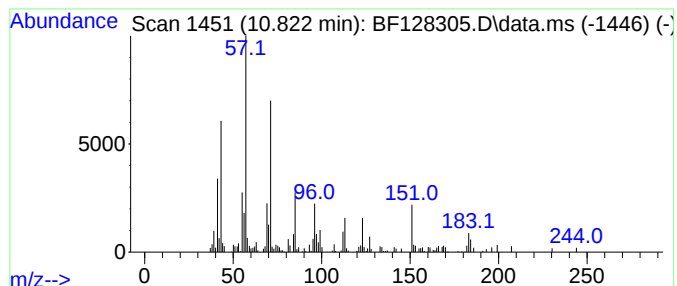
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Tridecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.822	4.14 ng	117954	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	60
2			Decane, 2-methyl-	156	C11H24	006975-98-0	53
3			Octadecane, 2,6-dimethyl-	282	C20H42	075163-97-2	50
4			2,6-Dimethyldecane	170	C12H26	013150-81-7	46
5			Pentadecane	212	C15H32	000629-62-9	43



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Misc :
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Instrument :
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ClientSampleId :
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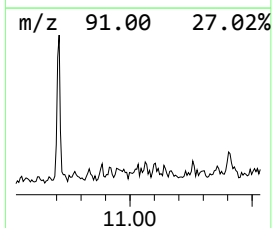
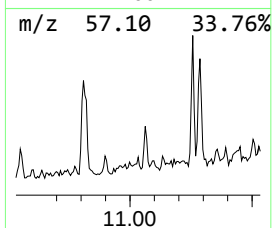
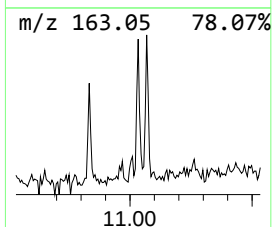
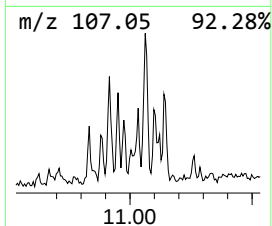
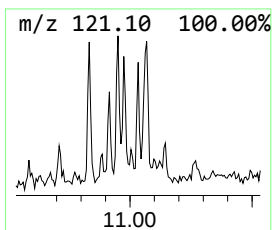
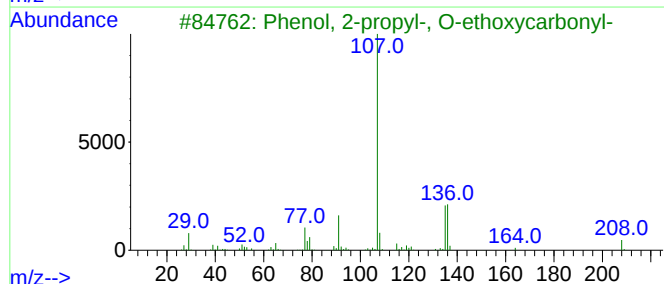
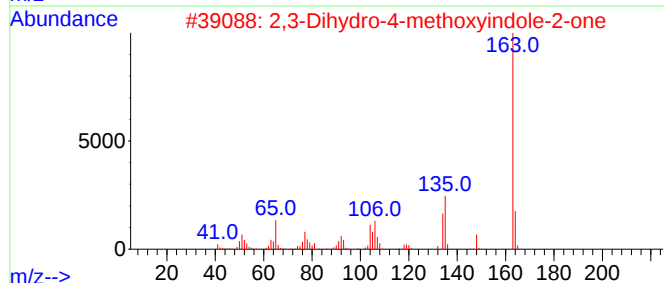
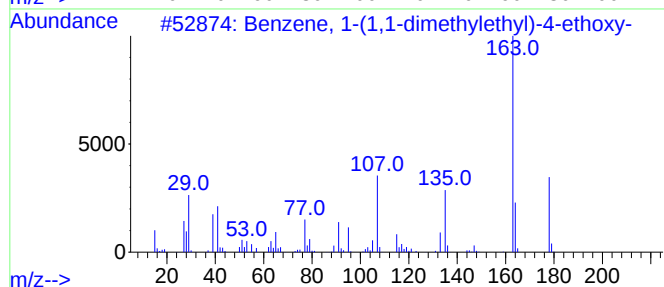
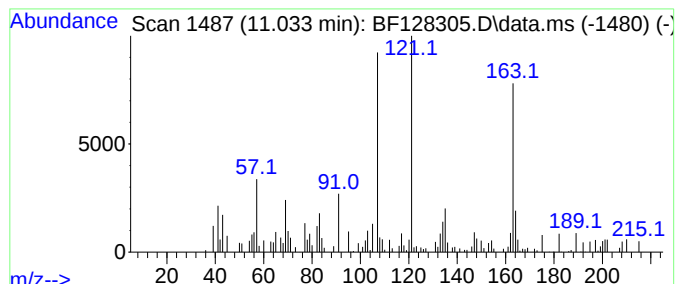
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown11.033 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.033	2.05 ng	58307	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-(1,1-dimethylethyl)-4...	178	C12H18O	017269-94-2	35
2			2,3-Dihydro-4-methoxyindole-2-one	163	C9H9NO2	007699-17-4	30
3			Phenol, 2-propyl-, O-ethoxycarbo...	208	C12H16O3	1000487-66-1	25
4			6-Fluoro-4-hydroxyquinoline	163	C9H6FN0	000391-78-6	25
5			3,5-Dimethyl-1-adamantanecarboxy...	208	C13H20O2	014670-94-1	25



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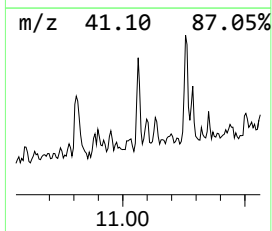
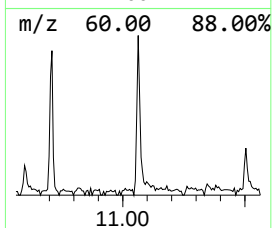
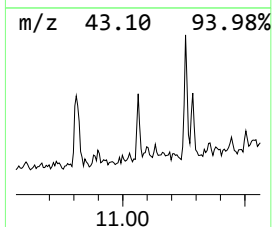
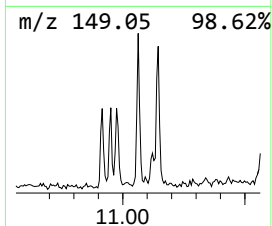
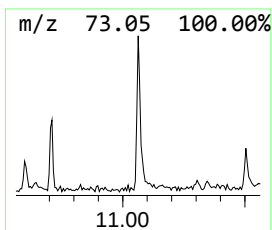
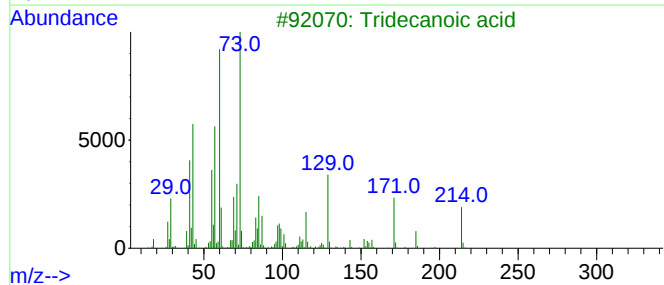
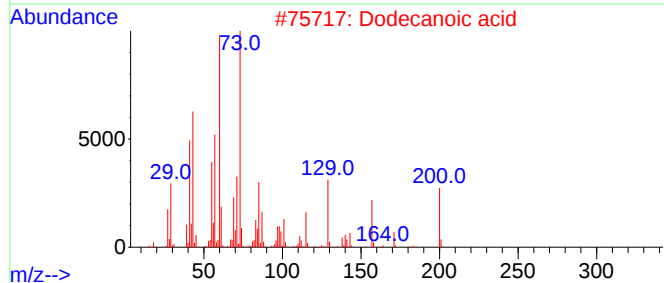
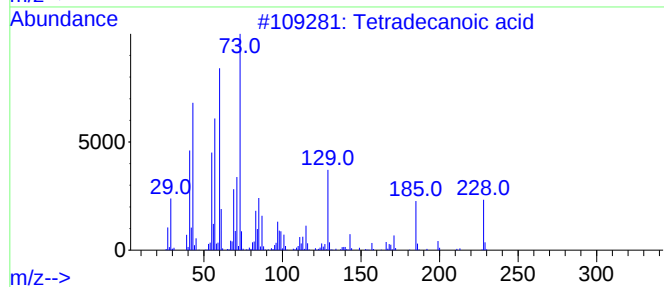
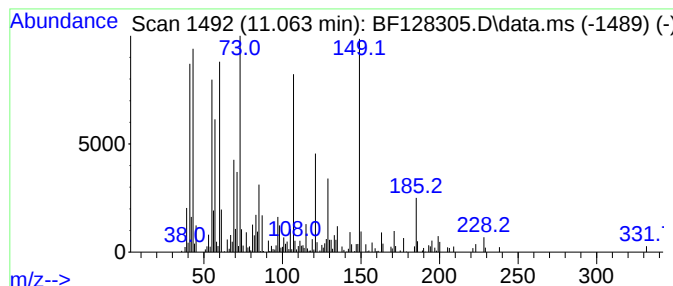
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tetradecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.063	3.42 ng	97368	Phenanthrene-d10		11.410	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Tetradecanoic acid		228	C14H28O2	000544-63-8	55
2	Dodecanoic acid		200	C12H24O2	000143-07-7	41
3	Tridecanoic acid		214	C13H26O2	000638-53-9	38
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	38
5	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	30



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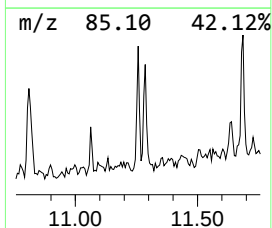
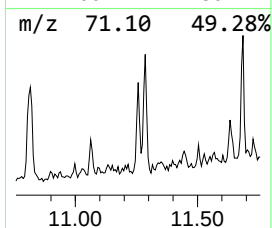
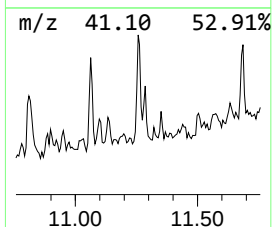
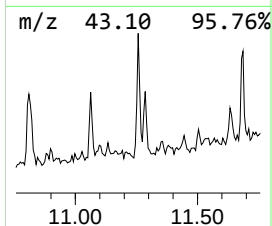
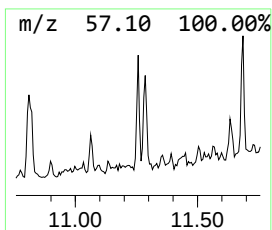
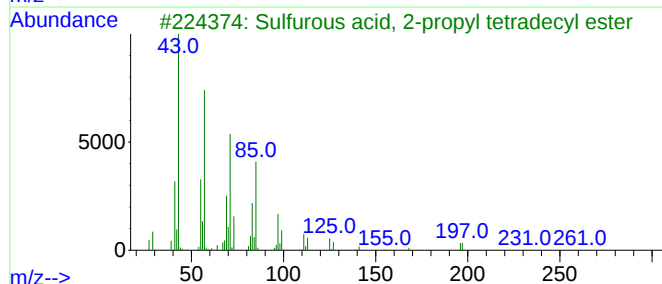
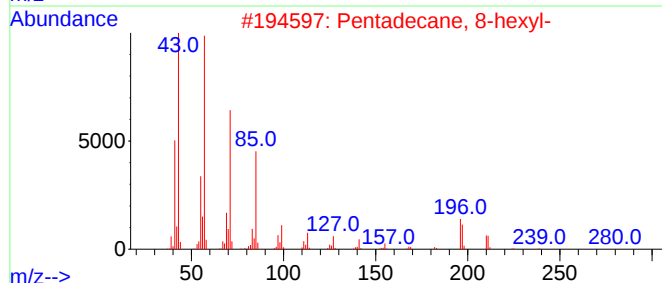
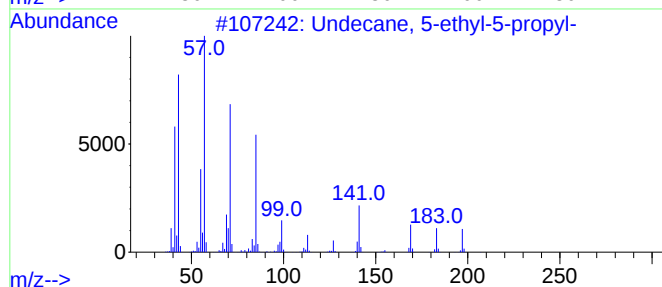
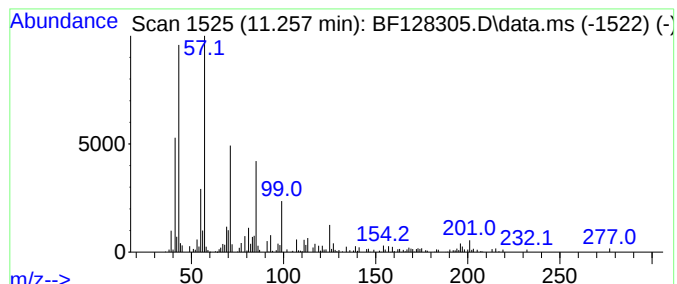
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Undecane, 5-ethyl-5-propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.257	3.64 ng	103601	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 5-ethyl-5-propyl-	226	C16H34	002755-07-9	64
2			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	64
3			Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1010309-12-5	58
4			Octacosane	394	C28H58	000630-02-4	58
5			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	58



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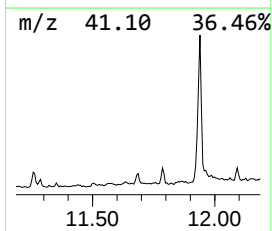
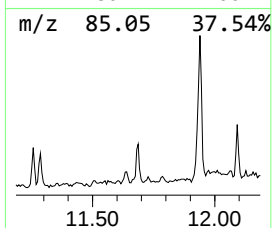
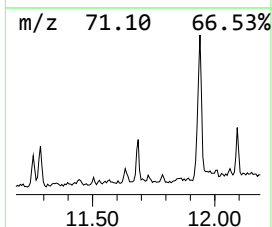
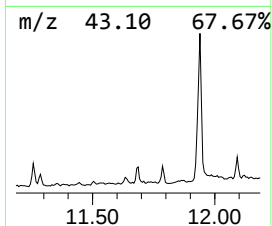
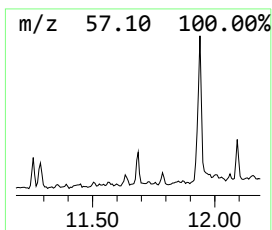
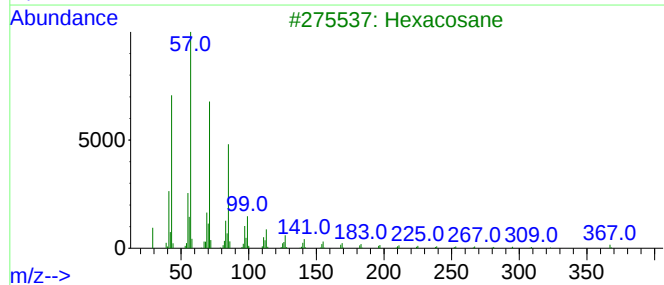
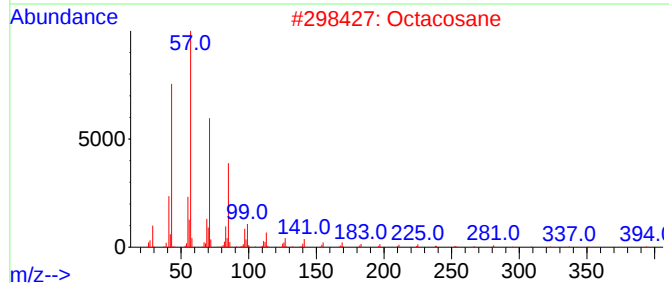
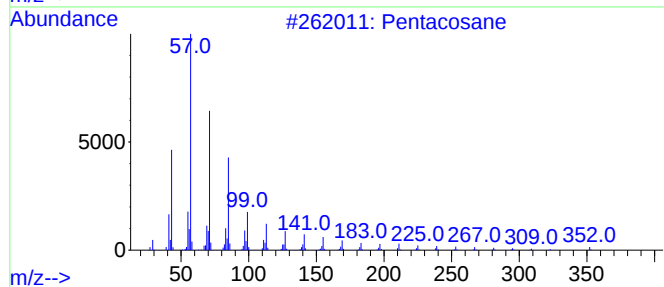
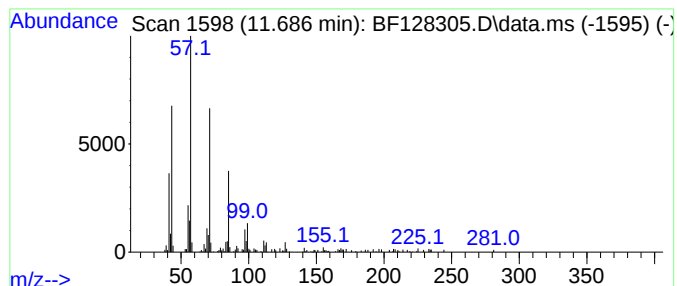
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ClientSampleId :
HR-02-051322

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.686	2.28 ng	64917	Phenanthrene-d10		11.410	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Pentacosane		352	C25H52	000629-99-2	86
2	Octacosane		394	C28H58	000630-02-4	83
3	Hexacosane		366	C26H54	000630-01-3	80
4	Eicosane, 10-methyl-		296	C21H44	054833-23-7	80
5	Tetracosane		338	C24H50	000646-31-1	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
Data File : BF128305.D
Acq On : 17 May 2022 22:07
Operator : CG\JU
Sample : N2856-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-02-051322

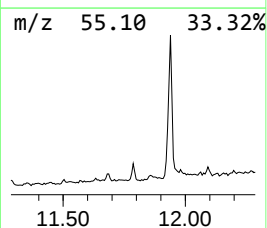
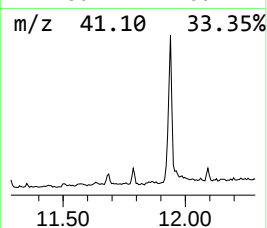
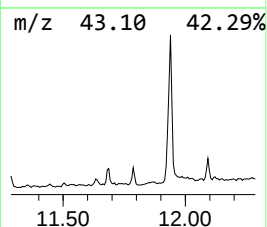
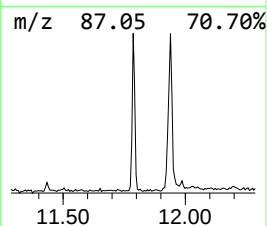
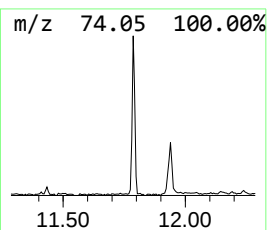
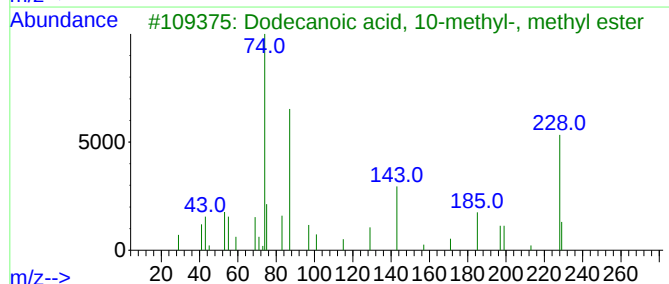
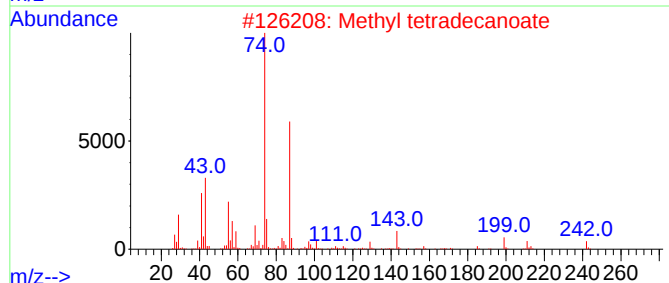
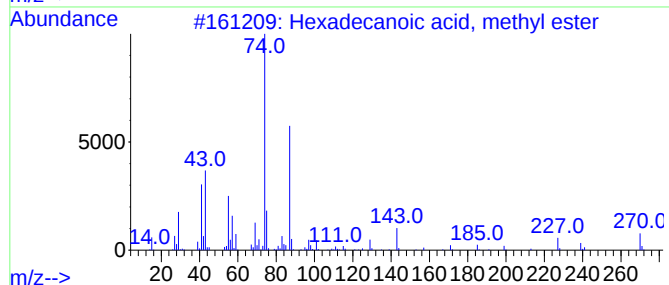
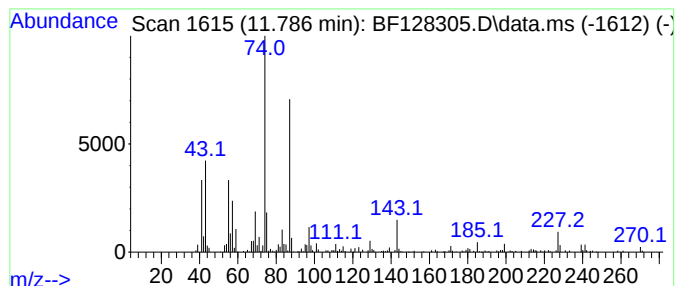
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.786	3.99 ng	113479	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	90
2			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
3			Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	83
4			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	81
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
Data File : BF128305.D
Acq On : 17 May 2022 22:07
Operator : CG\JU
Sample : N2856-01
Misc :
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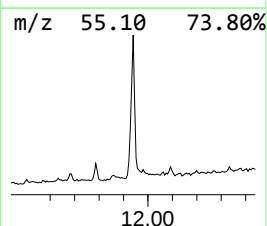
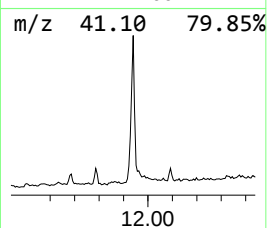
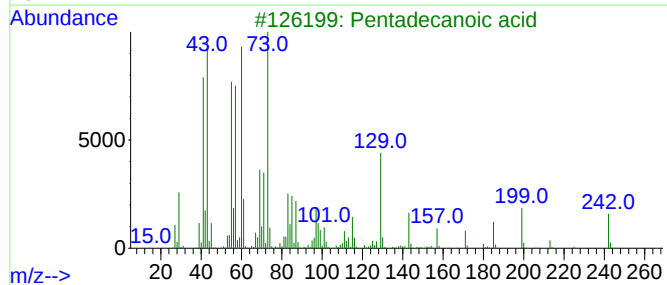
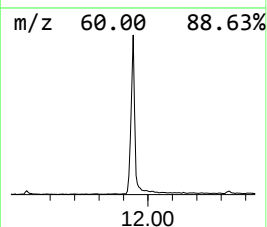
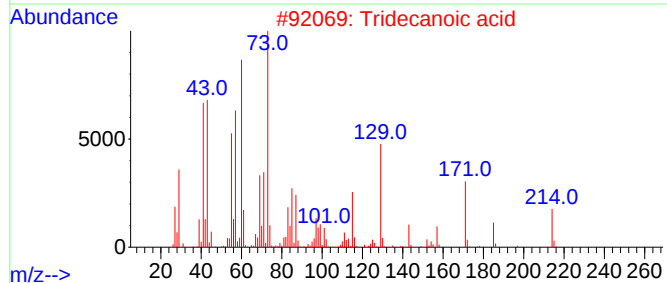
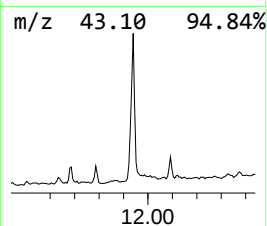
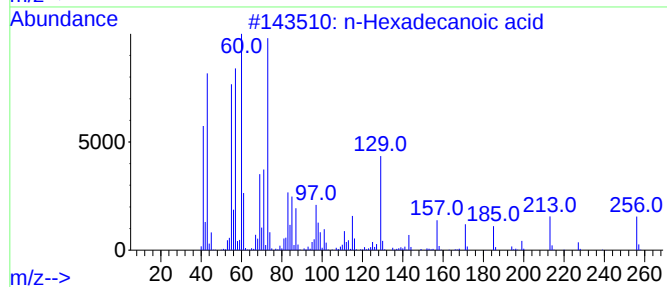
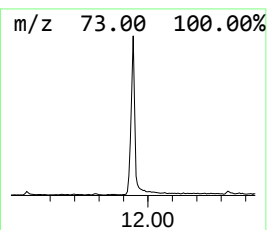
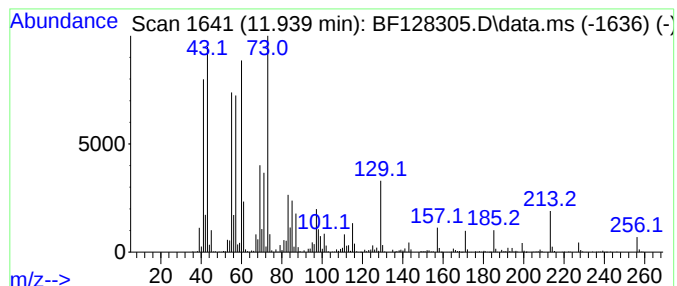
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.939	38.54 ng	1097070	Phenanthrene-d10		11.410	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	83
5	Nonanoic acid		158	C9H18O2	000112-05-0	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
Data File : BF128305.D
Acq On : 17 May 2022 22:07
Operator : CG\JU
Sample : N2856-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

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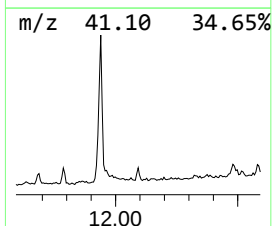
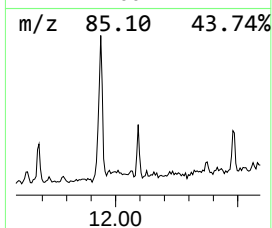
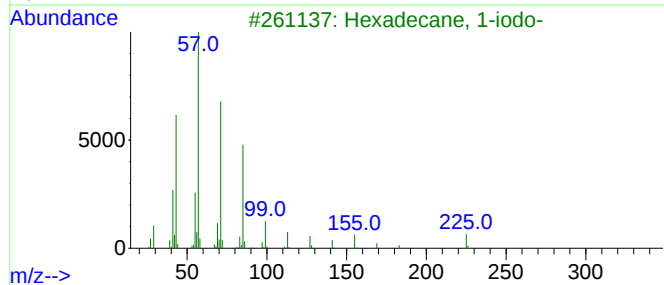
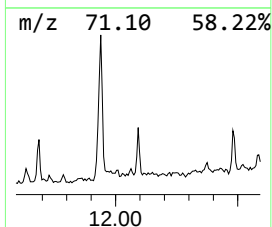
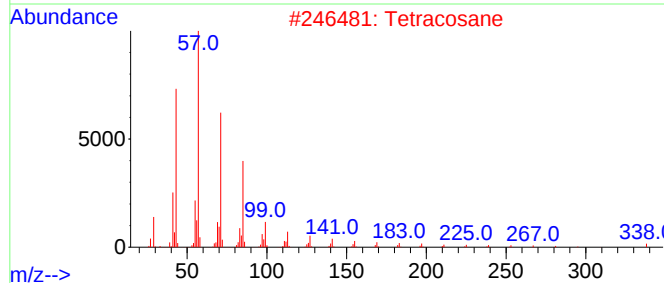
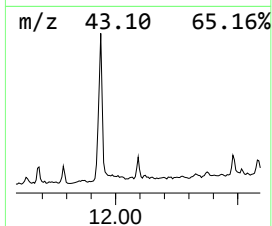
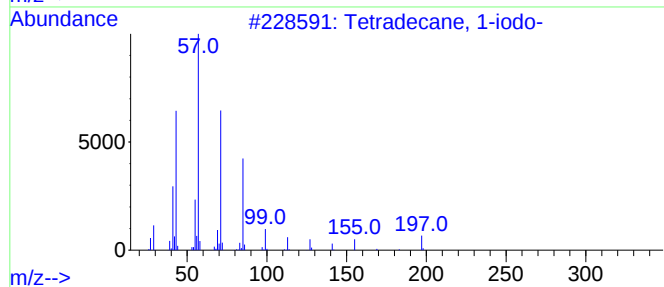
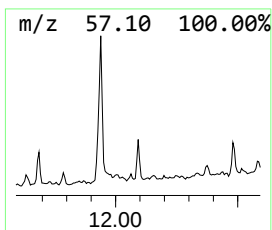
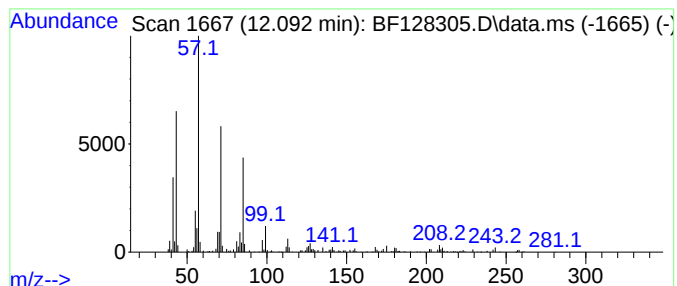
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetradecane, 1-iodo- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.092	2.31 ng	65630	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
2			Tetracosane	338	C24H50	000646-31-1	86
3			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	78
4			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	78
5			Eicosane, 10-methyl-	296	C21H44	054833-23-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
Data File : BF128305.D
Acq On : 17 May 2022 22:07
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Misc :
ALS Vial : 24 Sample Multiplier: 1

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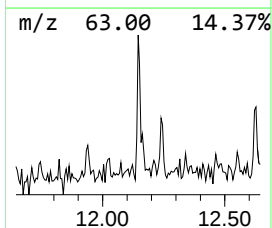
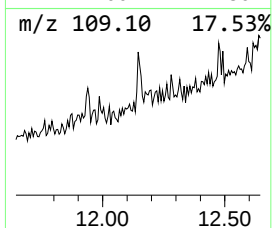
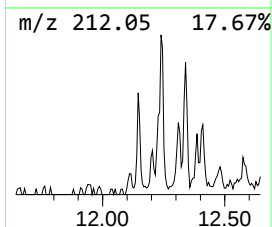
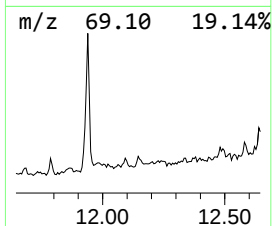
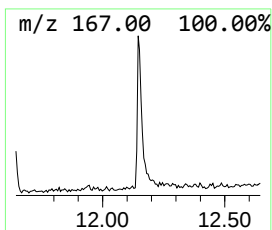
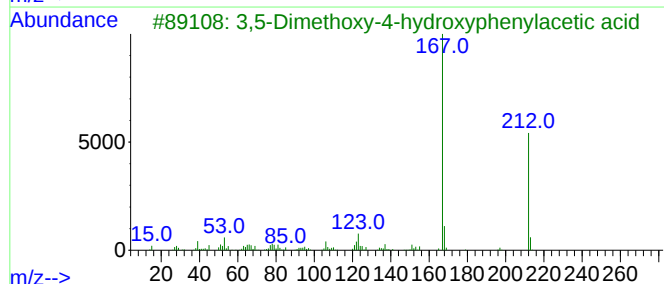
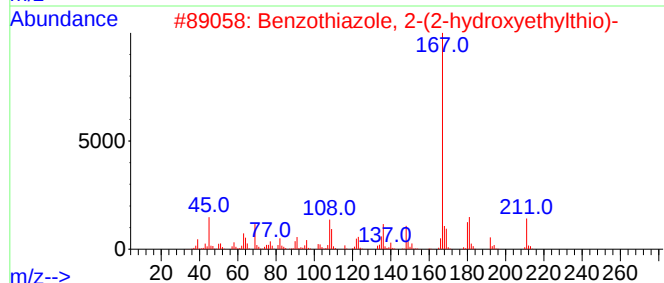
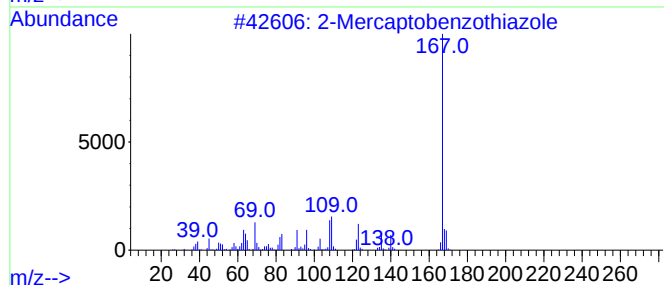
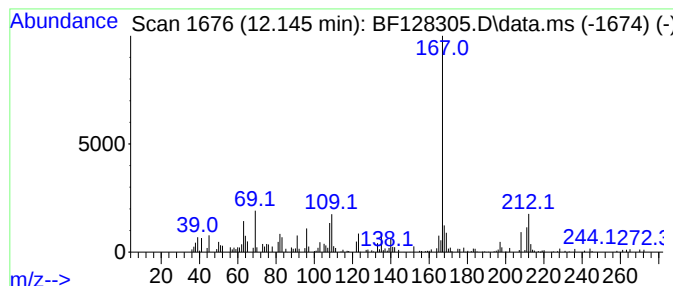
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-Mercaptobenzothiazole Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.145	2.88 ng	81867	Phenanthrene-d10	11.410

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	94
2		Benzothiazole, 2-(2-hydroxyethylthio)-	211	C9H9NOS2	004665-63-8	68
3		3,5-Dimethoxy-4-hydroxyphenylacetic acid	212	C10H12O5	004385-56-2	50
4		5-(2-Furyl)-4H-1,2,4-triazole-3-thione	167	C6H5N3OS	035771-65-4	50
5		Thioguanine	167	C5H5N5S	000154-42-7	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
Data File : BF128305.D
Acq On : 17 May 2022 22:07
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Sample : N2856-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
HR-02-051322

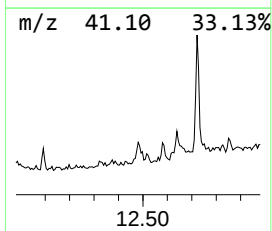
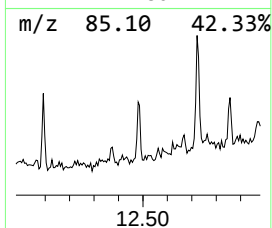
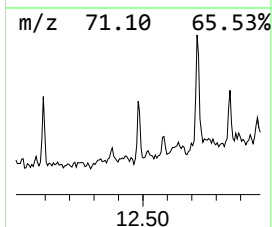
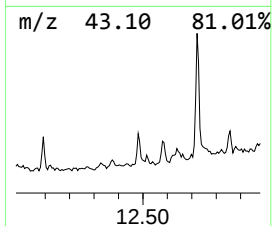
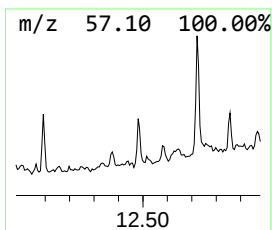
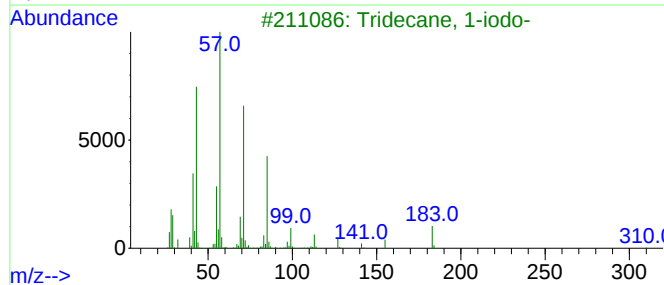
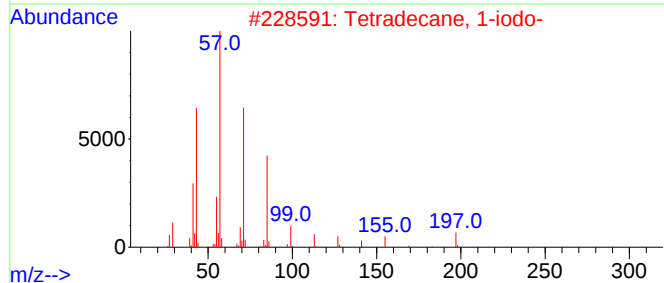
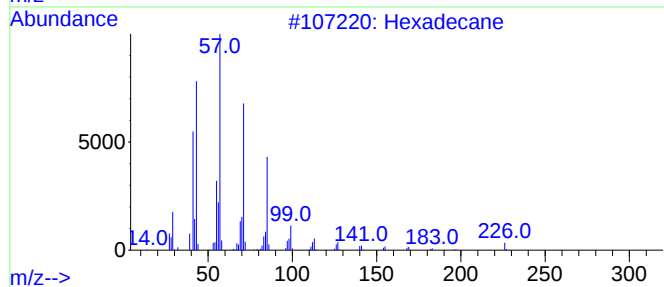
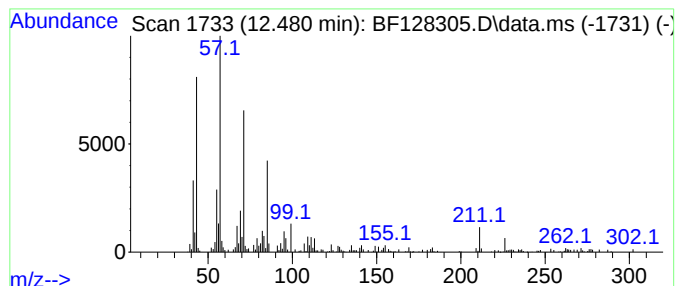
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.480	3.80 ng	108235	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	68
2			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	64
3			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64
4			Pentadecane	212	C15H32	000629-62-9	64
5			Eicosane	282	C20H42	000112-95-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
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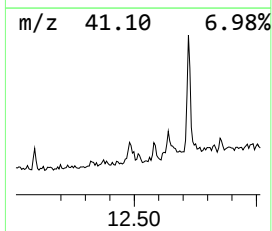
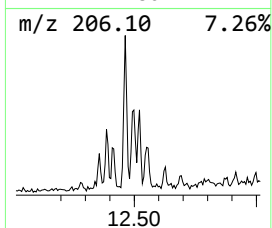
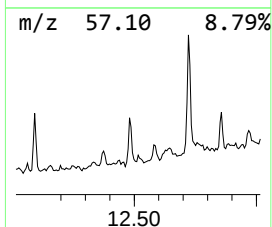
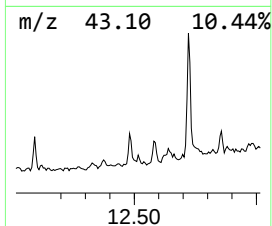
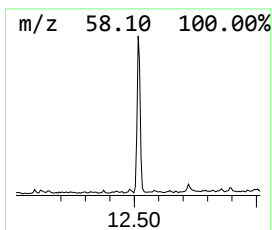
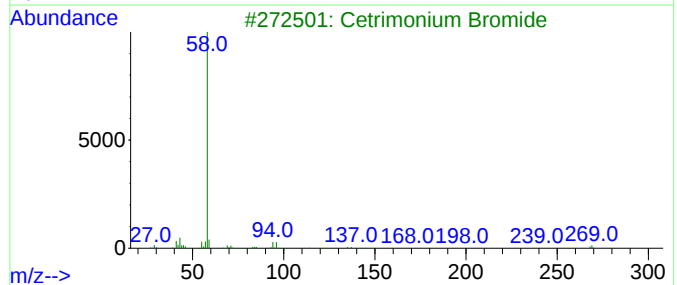
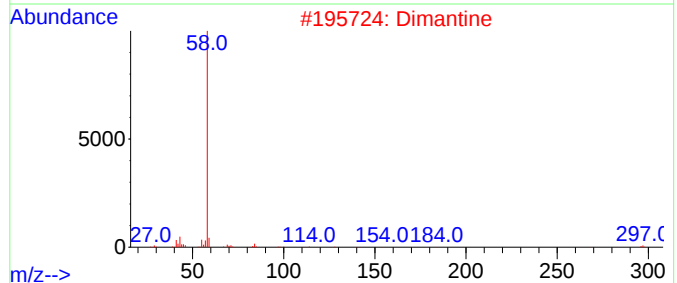
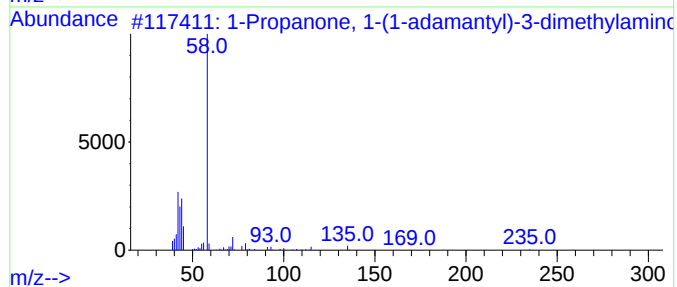
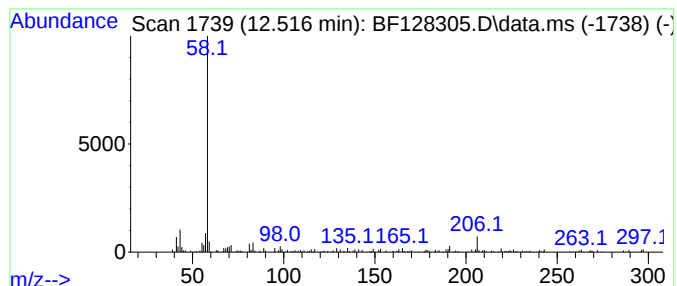
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Propanone, 1-(1-adamantyl)... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.516	2.11 ng	60031	Phenanthrene-d10		11.410	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Propanone, 1-(1-adamantyl)-3-d...		235	C15H25NO	031878-58-7	72
2	Dimantine		297	C20H43N	000124-28-7	72
3	Cetrimonium Bromide		363	C19H42BrN	000057-09-0	64
4	Methamphetamine		149	C10H15N	000537-46-2	64
5	N-[3-(Dimethylamino)-2,2-dimethy...		241	C13H27N3O	728932-41-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
Data File : BF128305.D
Acq On : 17 May 2022 22:07
Operator : CG\JU
Sample : N2856-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
HR-02-051322

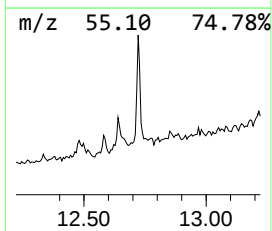
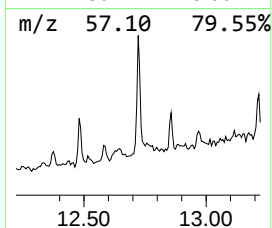
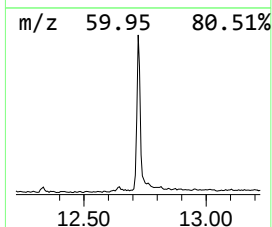
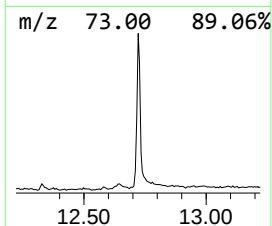
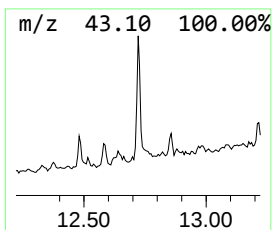
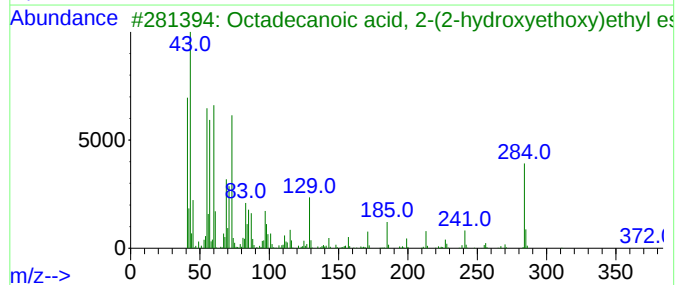
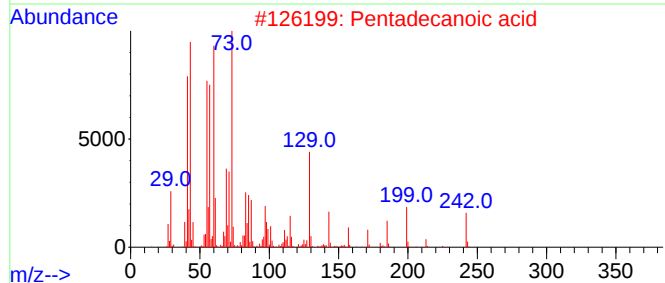
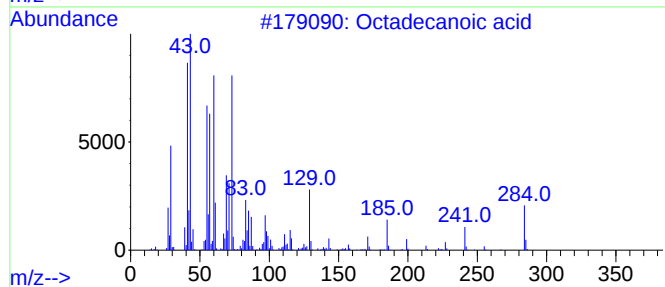
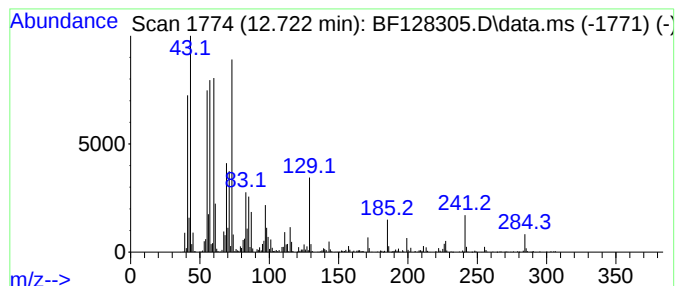
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.722	19.82 ng	564232	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
Data File : BF128305.D
Acq On : 17 May 2022 22:07
Operator : CG\JU
Sample : N2856-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-02-051322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.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
Tridecane	10.822	4.1	ng	117954	4	11.410	569334	20.0
unknown11.033	11.033	2.0	ng	58307	4	11.410	569334	20.0
Tetradecanoic acid	11.063	3.4	ng	97368	4	11.410	569334	20.0
Undecane, 5-eth...	11.257	3.6	ng	103601	4	11.410	569334	20.0
Pentacosane	11.686	2.3	ng	64917	4	11.410	569334	20.0
Hexadecanoic ac...	11.786	4.0	ng	113479	4	11.410	569334	20.0
n-Hexadecanoic ...	11.939	38.5	ng	1097070	4	11.410	569334	20.0
Tetradecane, 1-...	12.092	2.3	ng	65630	4	11.410	569334	20.0
2-Mercaptobenzo...	12.145	2.9	ng	81867	4	11.410	569334	20.0
Hexadecane	12.480	3.8	ng	108235	4	11.410	569334	20.0
1-Propanone, 1-...	12.516	2.1	ng	60031	4	11.410	569334	20.0
Octadecanoic acid	12.722	19.8	ng	564232	4	11.410	569334	20.0