

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050622\
 Data File : BF128125.D
 Acq On : 06 May 2022 15:36
 Operator : CG\JU
 Sample : N2712-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1

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-BF042222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128125.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.140	481	485	490	rVB	24717	29508	1.22%	0.177%
2	5.528	547	551	555	rBV	1832233	1799274	74.35%	10.818%
3	6.534	717	722	725	rBV	1917834	1844433	76.22%	11.090%
4	6.904	781	785	788	rBV	603671	477537	19.73%	2.871%
5	7.469	876	881	884	rBV	1324523	1230479	50.85%	7.398%
6	8.187	999	1003	1007	rBV	722948	617991	25.54%	3.716%
7	9.263	1180	1186	1189	rBV	2460427	2145224	88.65%	12.898%
8	9.945	1297	1302	1305	rBV	863623	718608	29.69%	4.321%
9	10.739	1432	1437	1440	rBV	1579943	1462572	60.44%	8.794%
10	11.439	1552	1556	1559	rBV	859940	773498	31.96%	4.651%
11	11.951	1637	1643	1646	rBV	86520	107548	4.44%	0.647%
12	12.104	1665	1669	1673	rBV	43597	54439	2.25%	0.327%
13	12.145	1673	1676	1682	rVB3	34037	53853	2.23%	0.324%
14	12.533	1733	1742	1743	rBV5	18872	44473	1.84%	0.267%
15	13.027	1821	1826	1829	rBV	2427433	2419966	100.00%	14.550%
16	13.922	1973	1978	1989	rBV4	94200	215881	8.92%	1.298%
17	14.045	1992	1999	2002	rBV3	81941	181163	7.49%	1.089%
18	14.080	2002	2005	2009	rVB	732483	710759	29.37%	4.274%
19	14.227	2026	2030	2032	rBV	29038	30576	1.26%	0.184%
20	14.533	2079	2082	2084	rBV	29729	26545	1.10%	0.160%
21	14.616	2084	2096	2111	rBV2	210410	681441	28.16%	4.097%
22	14.845	2132	2135	2137	rBV	35641	45248	1.87%	0.272%
23	14.874	2137	2140	2153	rVB5	61983	151279	6.25%	0.910%
24	15.192	2191	2194	2201	rVB	41737	57773	2.39%	0.347%
25	15.357	2216	2222	2232	rVB5	37440	97137	4.01%	0.584%
26	15.586	2255	2261	2266	rVB	410353	529175	21.87%	3.182%
27	15.774	2290	2293	2303	rVB4	38814	98367	4.06%	0.591%
28	16.033	2335	2337	2343	rVB2	24368	26892	1.11%	0.162%

Sum of corrected areas: 16631639

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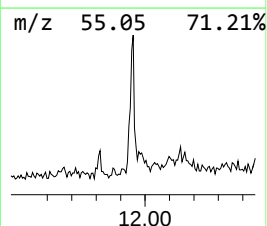
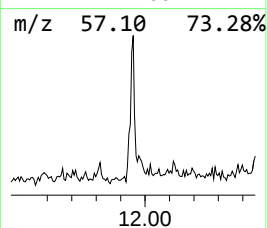
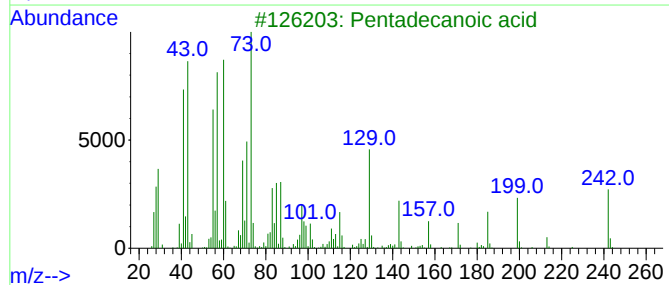
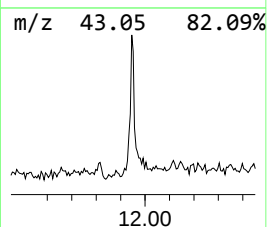
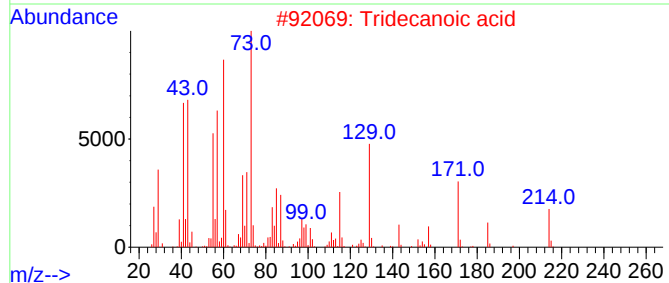
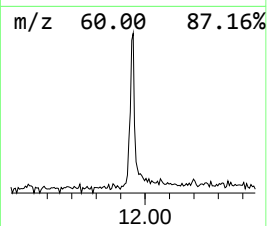
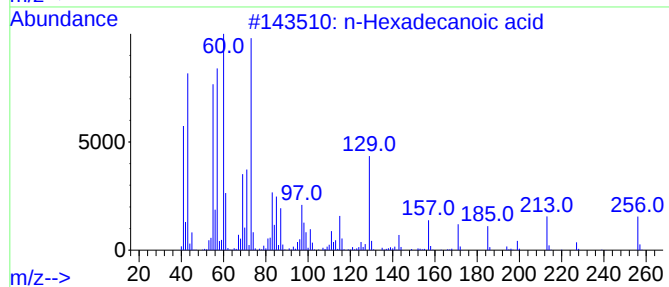
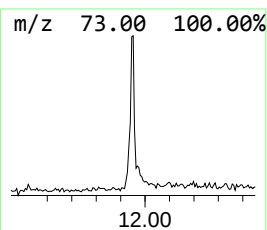
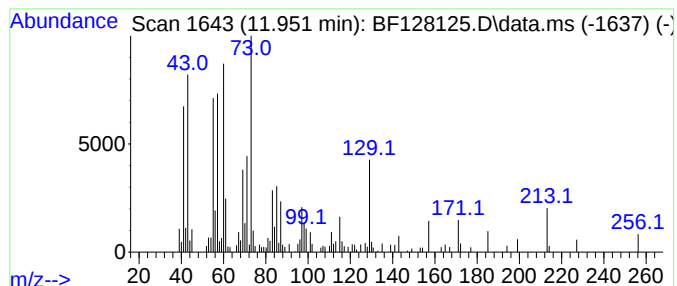
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	2.78 ng	107548	Phenanthrene-d10	11.439

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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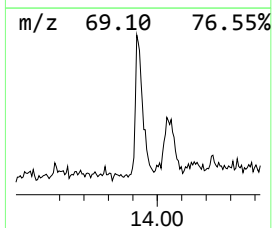
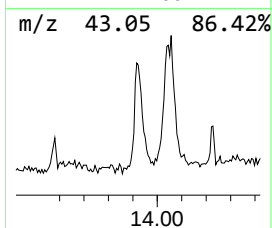
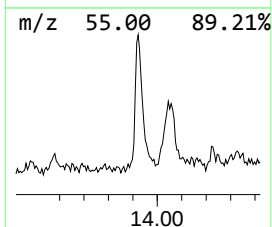
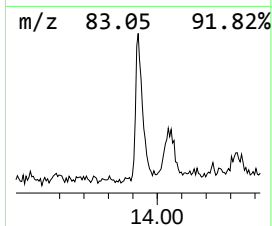
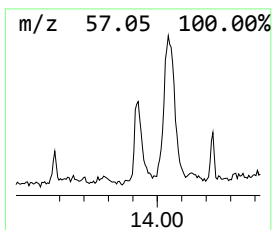
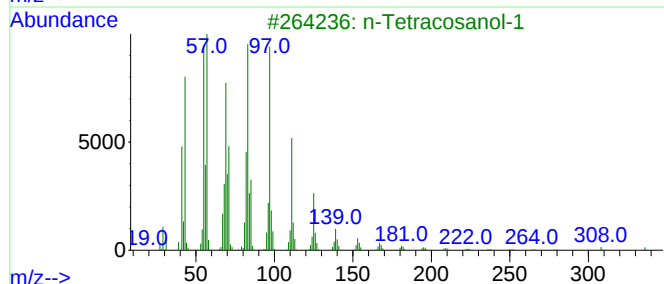
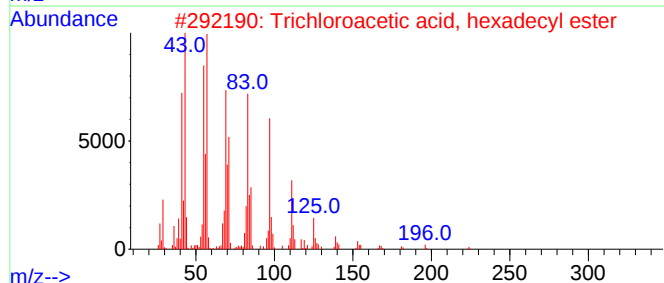
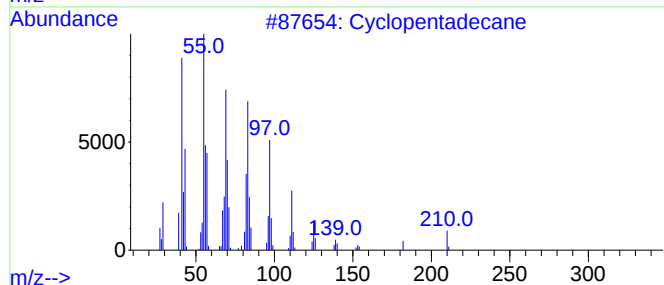
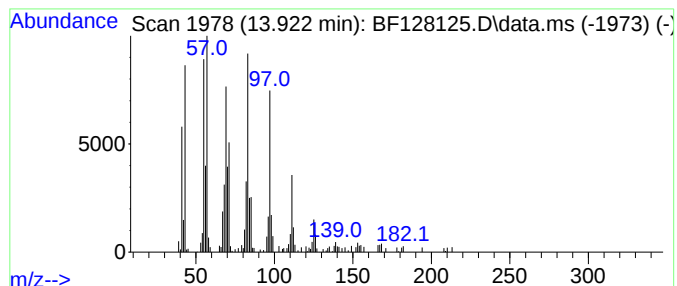
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Peak Number 2 Cyclopentadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.922	6.07 ng	215881	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	97
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4			Behenic alcohol	326	C22H46O	000661-19-8	94
5			1-Tricosene	322	C23H46	018835-32-0	94



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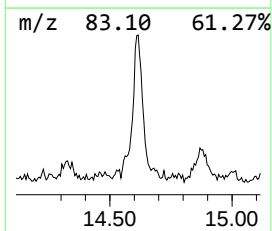
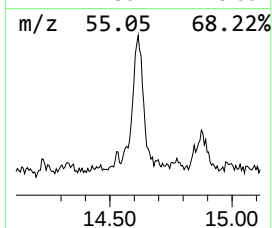
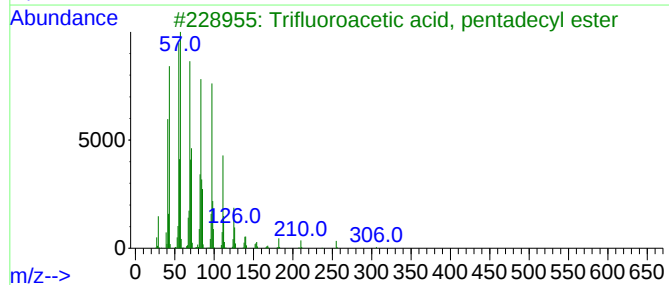
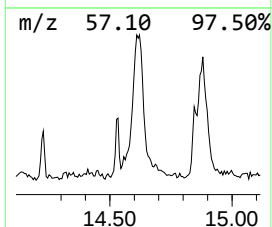
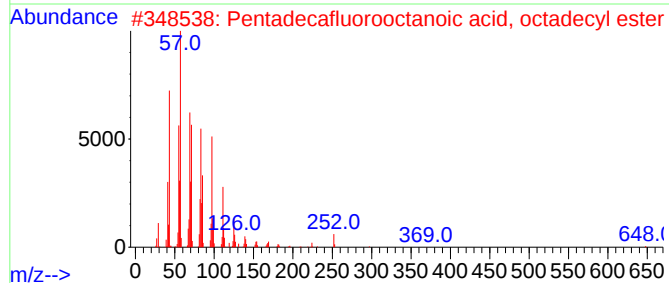
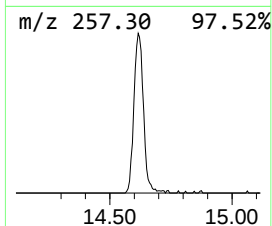
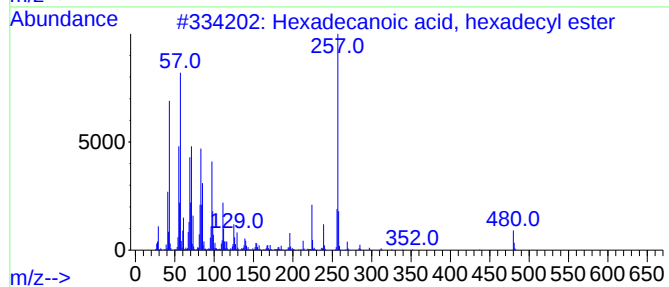
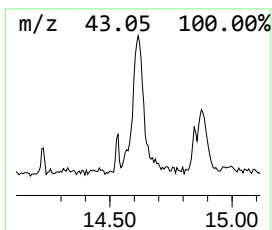
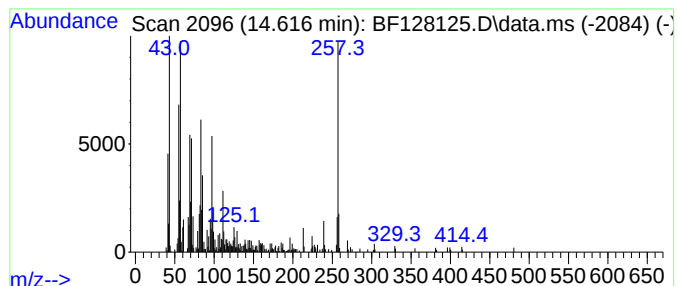
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Peak Number 3 Hexadecanoic acid, hexadecy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.616	19.18 ng	681441	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, hexadecyl ester	480	C32H64O2	000540-10-3	96
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
3			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	87
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	83
5			Hexadecanoic acid, tetradecyl ester	452	C30H60O2	004536-26-9	81



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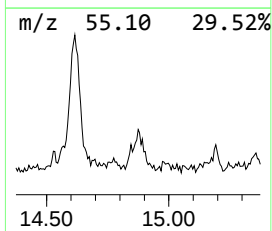
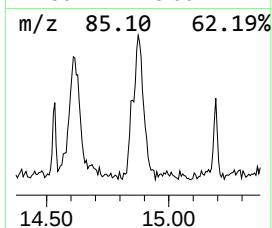
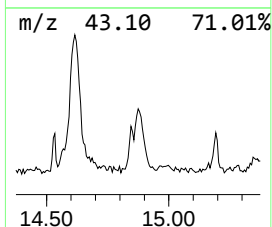
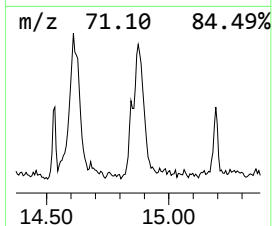
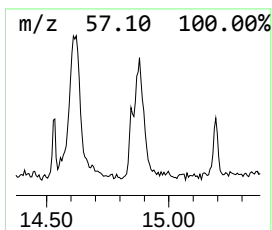
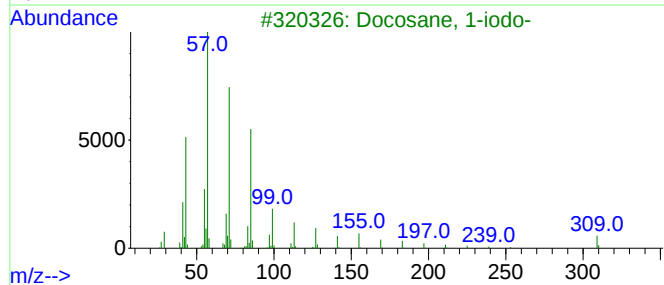
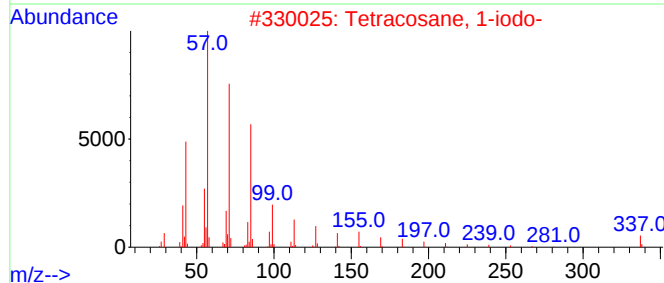
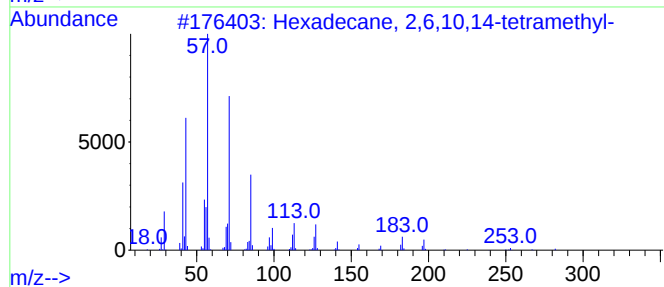
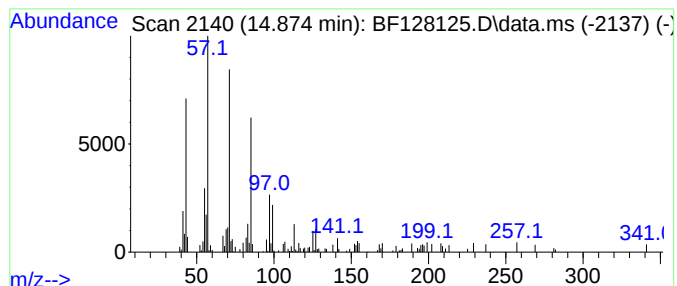
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Peak Number 4 Hexadecane, 2,6,10,14-tetra... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.874	5.72 ng	151279	Perylene-d12	15.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	83
2			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	74
3			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	74
4			Hexacosane	366	C26H54	000630-01-3	72
5			Tridecane, 3-methyl-	198	C14H30	006418-41-3	72



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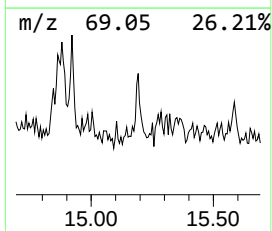
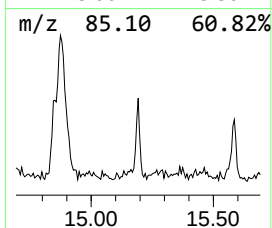
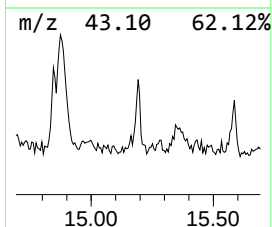
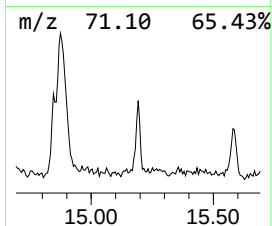
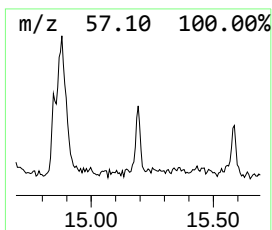
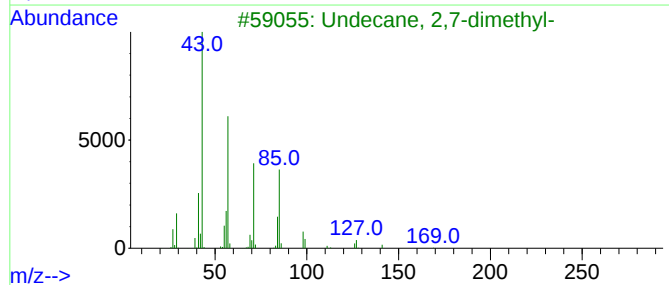
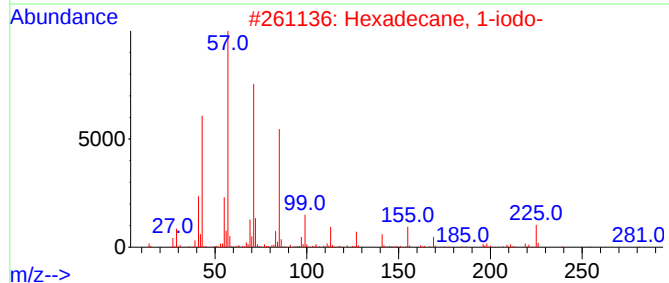
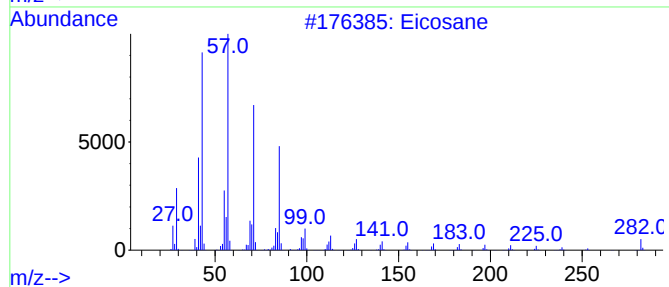
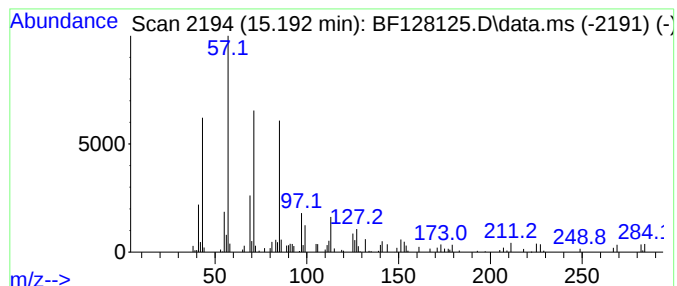
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Peak Number 5 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.192	2.18 ng	57773	Perylene-d12	15.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	86
2			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	72
3			Undecane, 2,7-dimethyl-	184	C13H28	017301-24-5	59
4			Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	59
5			Decane, 1-iodo-	268	C10H21I	002050-77-3	58



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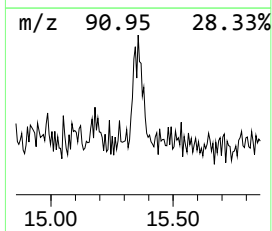
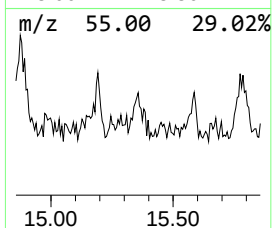
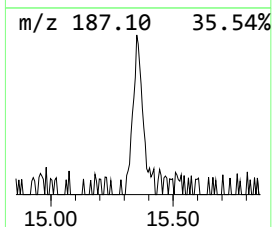
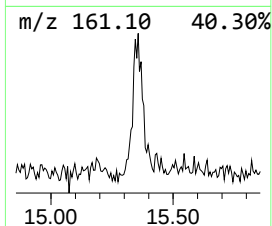
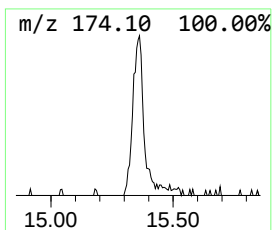
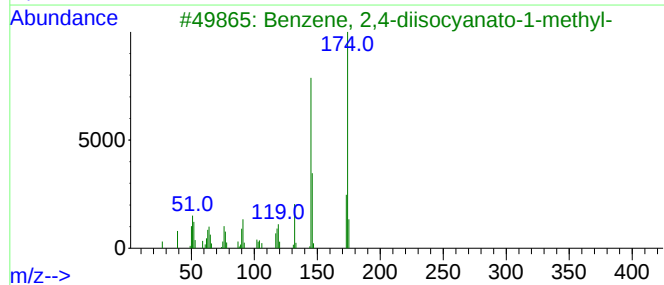
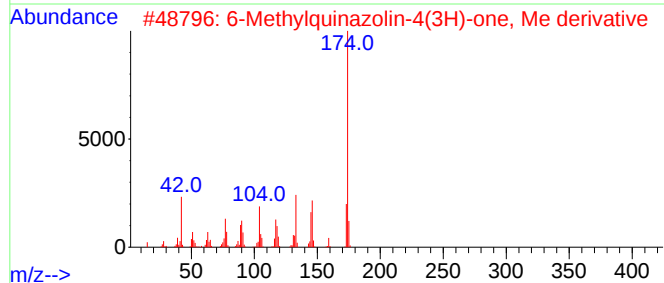
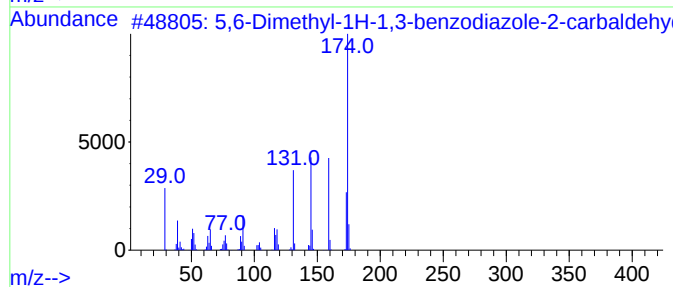
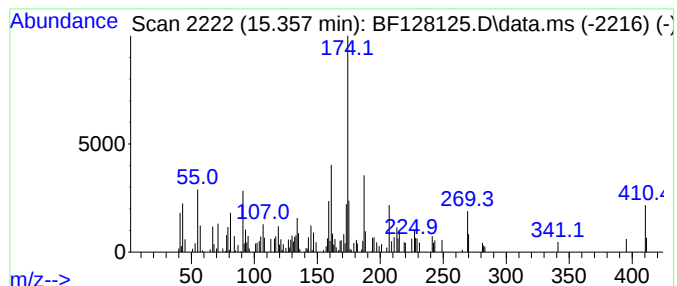
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown15.357 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.357	3.67 ng	97137	Perylene-d12	15.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5,6-Dimethyl-1H-1,3-benzodiazole...	174	C10H10N2O	920484-85-1	38
2			6-Methylquinazolin-4(3H)-one, Me...	174	C10H10N2O	1010504-83-5	35
3			Benzene, 2,4-diisocyanato-1-methyl-	174	C9H6N2O2	000584-84-9	27
4			2-(Aminomethyl)-4-methylpentanoi...	361	C16H39N02Si3	1000501-34-5	27
5			5-Methyl-5,8-dihydro-1,4-naphtho...	174	C11H10O2	086759-40-2	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050622\
Data File : BF128125.D
Acq On : 06 May 2022 15:36
Operator : CG\JU
Sample : N2712-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

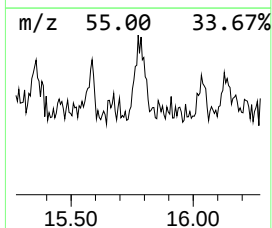
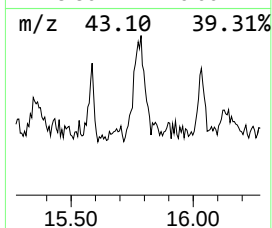
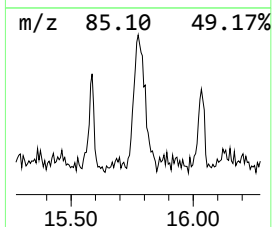
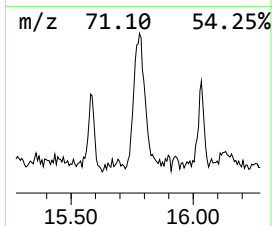
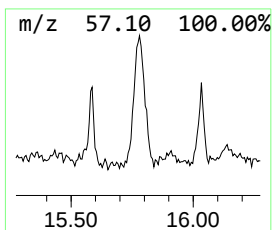
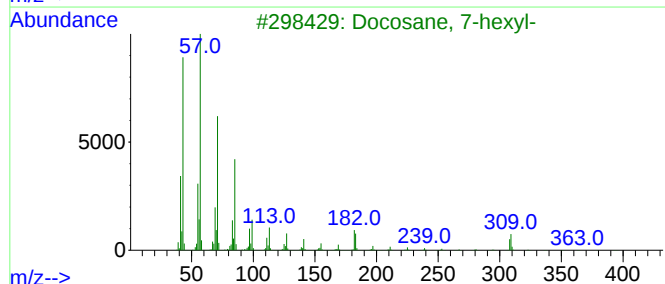
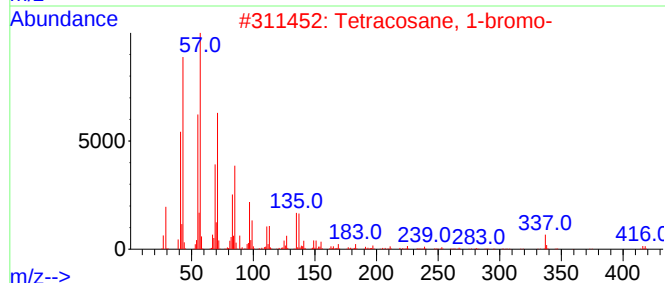
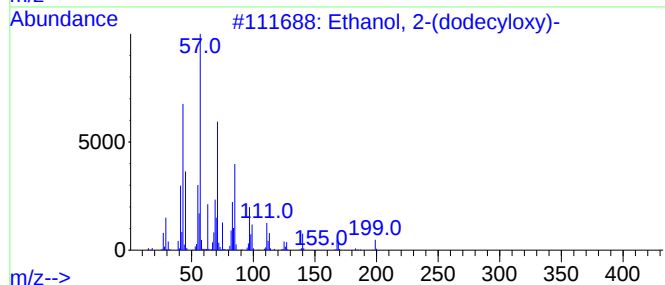
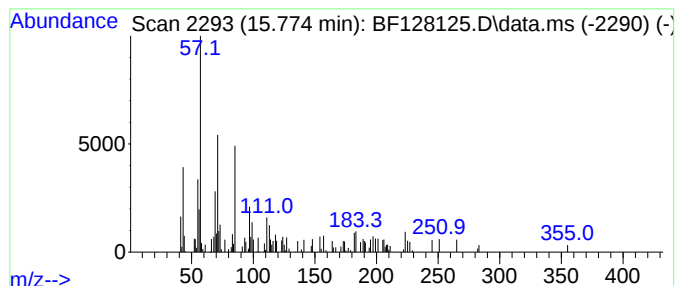
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Ethanol, 2-(dodecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.774	3.72 ng	98367	Perylene-d12	15.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	50
2			Tetracosane, 1-bromo-	416	C24H49Br	006946-24-3	50
3			Docosane, 7-hexyl-	394	C28H58	055373-86-9	50
4			Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	50
5			Carbonic acid, di(decyl) ester	342	C21H42O3	1000383-15-9	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050622\
Data File : BF128125.D
Acq On : 06 May 2022 15:36
Operator : CG\JU
Sample : N2712-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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 ...	11.951	2.8	ng	107548	4	11.439	773498	20.0
Cyclopentadecane	13.922	6.1	ng	215881	5	14.080	710759	20.0
Hexadecanoic ac...	14.616	19.2	ng	681441	5	14.080	710759	20.0
Hexadecane, 2,6...	14.874	5.7	ng	151279	6	15.586	529175	20.0
Eicosane	15.192	2.2	ng	57773	6	15.586	529175	20.0
unknown15.357	15.357	3.7	ng	97137	6	15.586	529175	20.0
Ethanol, 2-(dod...	15.774	3.7	ng	98367	6	15.586	529175	20.0