

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030822\
 Data File : BF127255.D
 Acq On : 08 Mar 2022 13:34
 Operator : CG\JU
 Sample : N1763-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 23-24-SAMPLE-LOCATION-12

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-BF021622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127255.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.110	476	480	487	rVB	20279	27159	1.24%	0.180%
2	5.504	543	547	550	rBV	2379167	2120640	96.94%	14.088%
3	6.510	713	718	721	rBV	2238972	2187483	100.00%	14.532%
4	6.875	777	780	784	rBV	731980	583033	26.65%	3.873%
5	7.439	871	876	879	rBV	1464322	1476883	67.52%	9.811%
6	7.604	901	904	908	rVB	27836	27022	1.24%	0.180%
7	8.157	994	998	1002	rBV	741532	653674	29.88%	4.342%
8	8.739	1091	1097	1100	rVB	36915	29347	1.34%	0.195%
9	9.233	1176	1181	1184	rBV	2426757	2164616	98.95%	14.380%
10	9.304	1189	1193	1196	rVV	92633	74602	3.41%	0.496%
11	9.833	1280	1283	1288	rVB	88561	72846	3.33%	0.484%
12	9.922	1293	1298	1301	rBV	783204	705256	32.24%	4.685%
13	10.063	1319	1322	1325	rBV3	17399	24291	1.11%	0.161%
14	10.339	1366	1369	1371	rVB	86152	71692	3.28%	0.476%
15	10.551	1400	1405	1408	rBV2	27659	44819	2.05%	0.298%
16	10.710	1428	1432	1436	rBV	1562157	1390024	63.54%	9.234%
17	10.810	1446	1449	1453	rBV	79349	75659	3.46%	0.503%
18	11.263	1522	1526	1528	rBV	52020	52357	2.39%	0.348%
19	11.286	1528	1530	1537	rVB5	27229	38312	1.75%	0.255%
20	11.410	1548	1551	1554	rBV	740087	621465	28.41%	4.128%
21	11.686	1596	1598	1604	rVB	50667	48150	2.20%	0.320%
22	11.757	1606	1610	1613	rVV	32985	52361	2.39%	0.348%
23	11.792	1613	1616	1619	rVB	66952	57896	2.65%	0.385%
24	12.098	1665	1668	1671	rBV	30903	27230	1.24%	0.181%
25	12.480	1730	1733	1735	rBV2	75966	69692	3.19%	0.463%
26	12.998	1817	1821	1824	rBV	1668229	1353052	61.85%	8.988%
27	13.874	1967	1970	1974	rBV3	60732	63815	2.92%	0.424%
28	13.921	1976	1978	1988	rVB4	54204	101545	4.64%	0.675%
29	14.057	1998	2001	2005	rVB	397330	345762	15.81%	2.297%
30	14.810	2126	2129	2136	rVB2	57876	70507	3.22%	0.468%
31	15.551	2251	2255	2263	rVB2	301005	422104	19.30%	2.804%

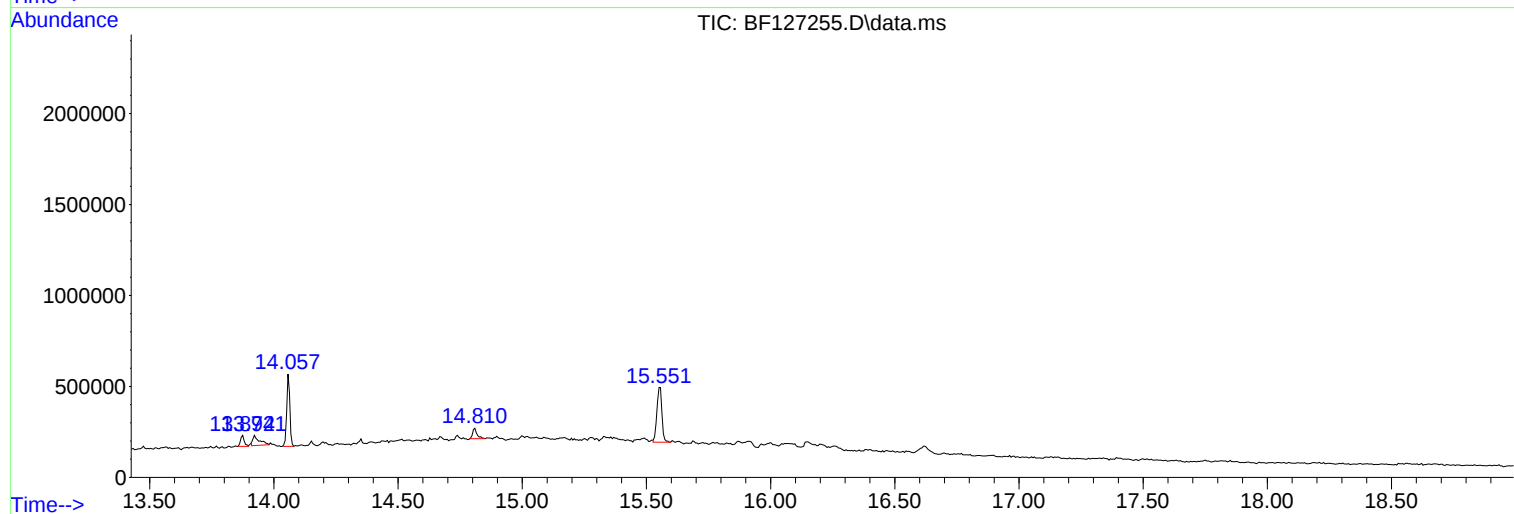
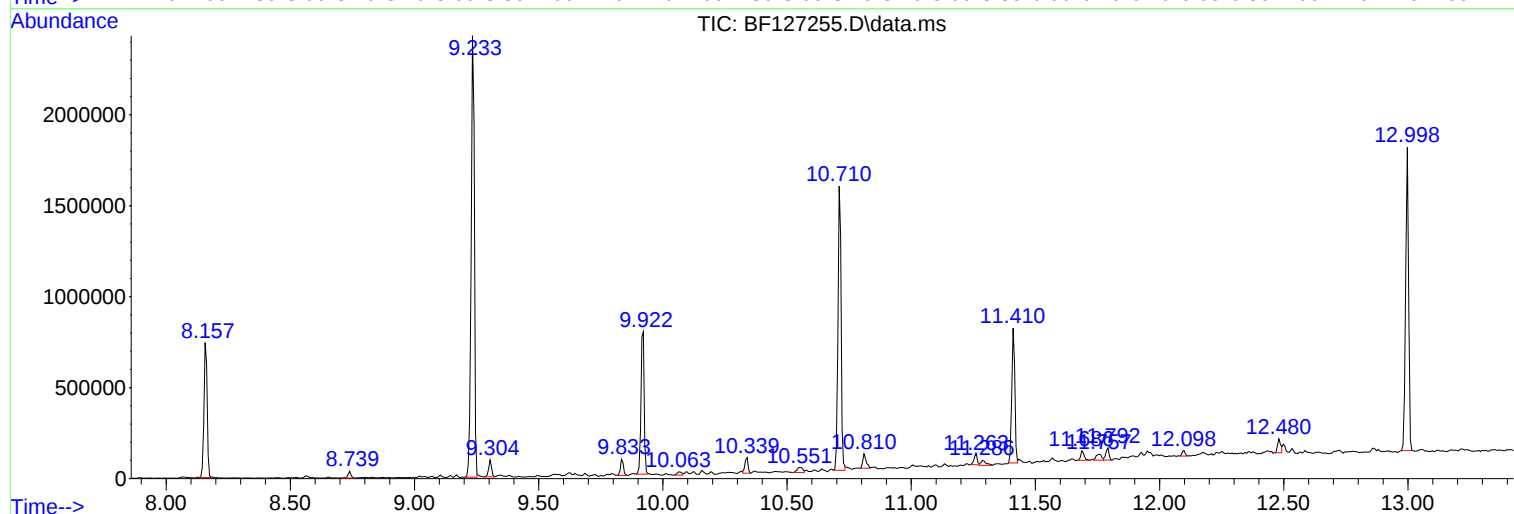
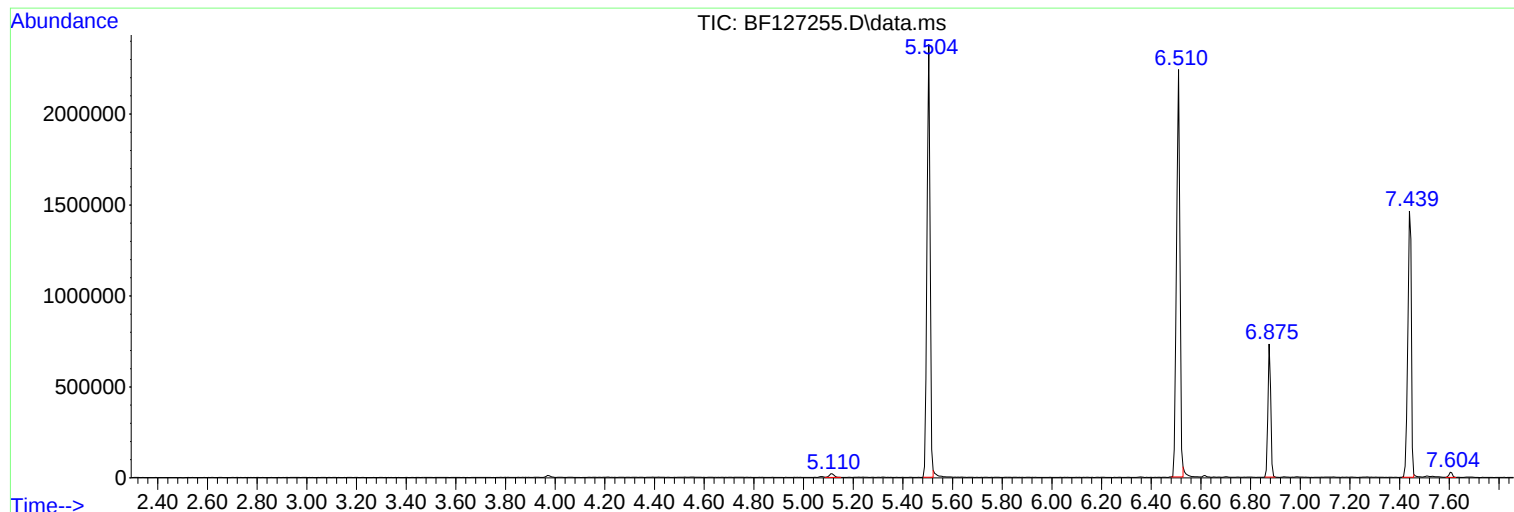
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ClientSampleId :
23-24-SAMPLE-LOCATION-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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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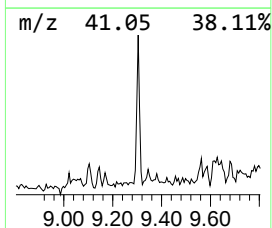
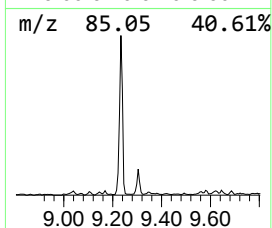
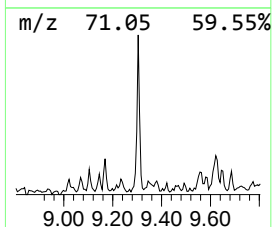
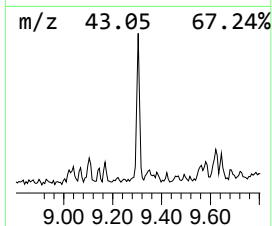
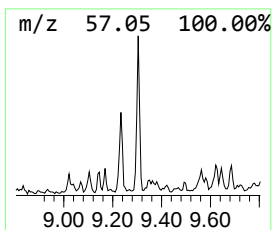
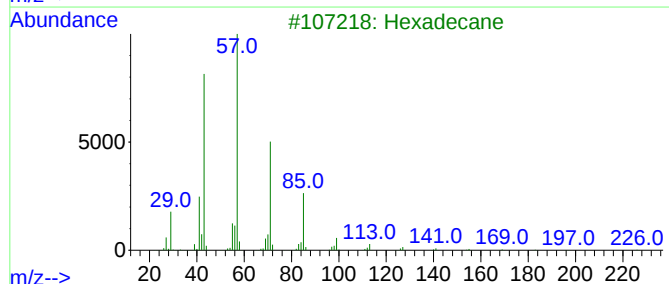
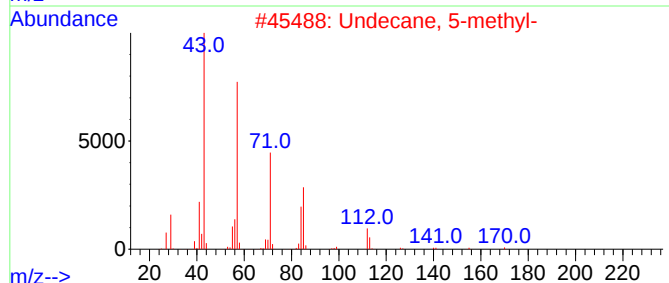
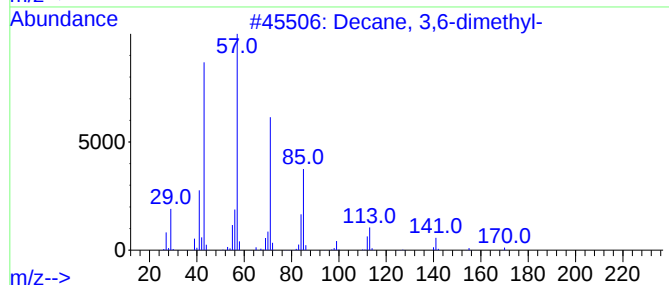
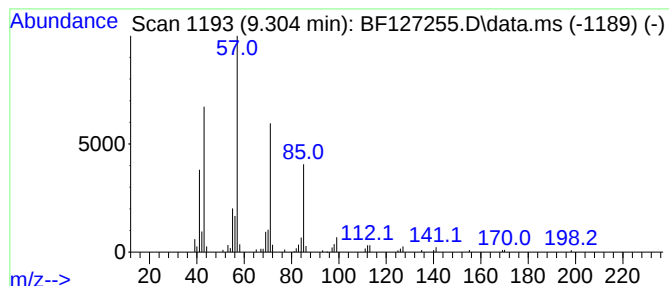
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Decane, 3,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.304	2.12 ng	74602	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	87
2			Undecane, 5-methyl-	170	C12H26	001632-70-8	86
3			Hexadecane	226	C16H34	000544-76-3	80
4			Dodecane	170	C12H26	000112-40-3	80
5			Tetradecane	198	C14H30	000629-59-4	64



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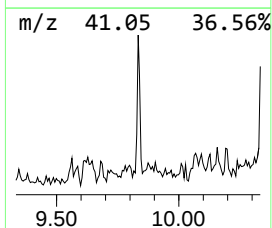
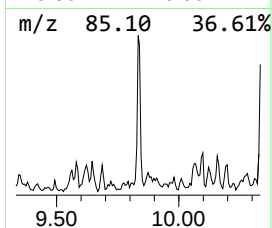
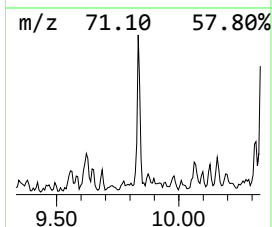
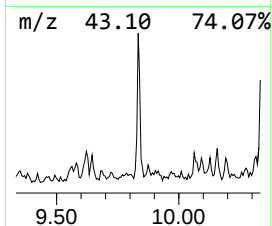
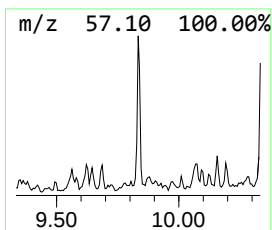
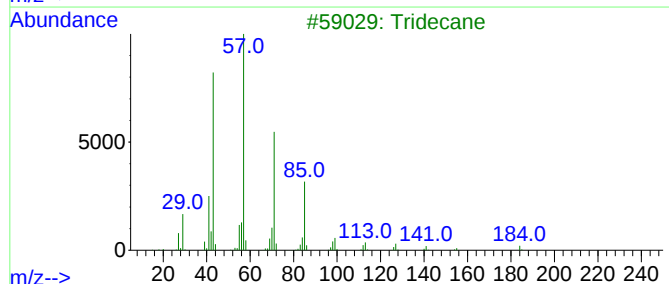
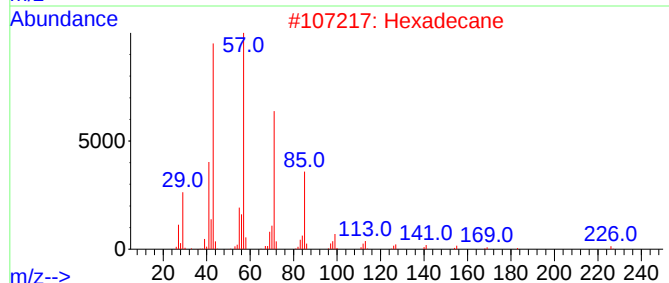
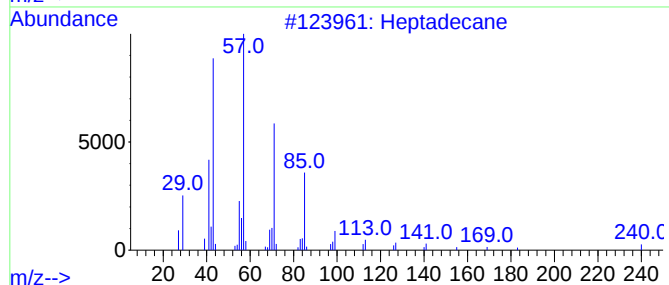
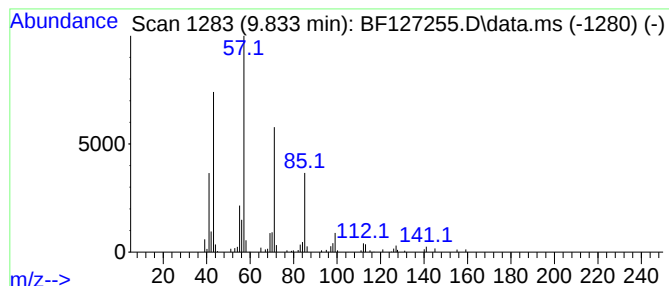
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Peak Number 2 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.833	2.07 ng	72846	Acenaphthene-d10	9.922

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	91
2		Hexadecane	226	C16H34	000544-76-3	91
3		Tridecane	184	C13H28	000629-50-5	90
4		Pentadecane	212	C15H32	000629-62-9	90
5		Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	80



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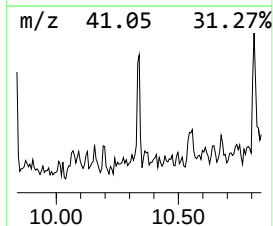
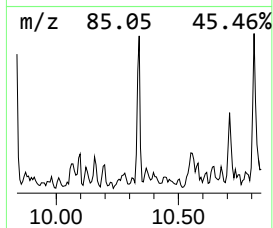
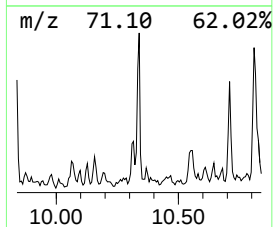
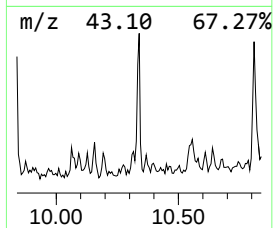
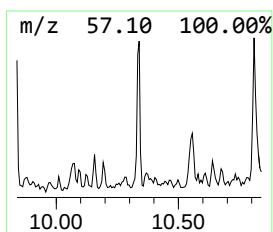
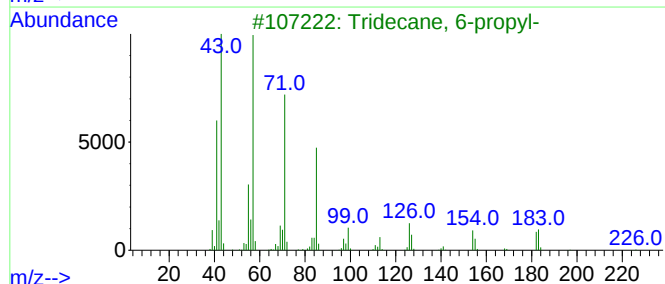
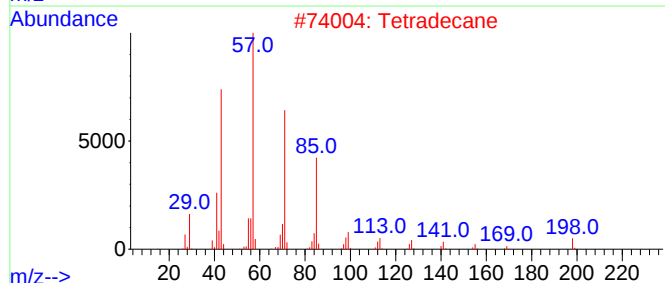
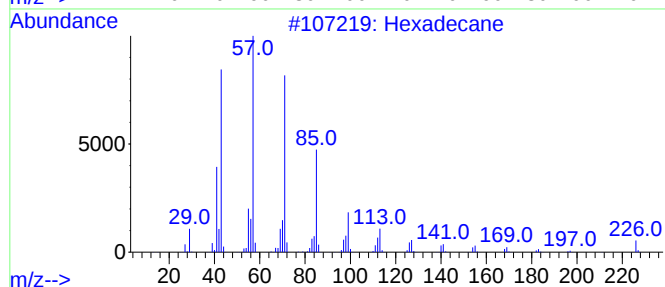
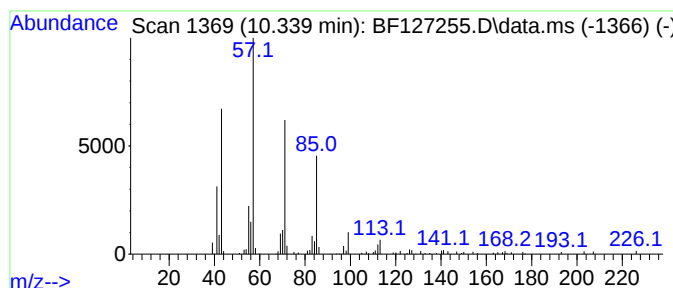
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.339	2.03 ng	71692	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	91
2			Tetradecane	198	C14H30	000629-59-4	86
3			Tridecane, 6-propyl-	226	C16H34	055045-10-8	83
4			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	83
5			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	78



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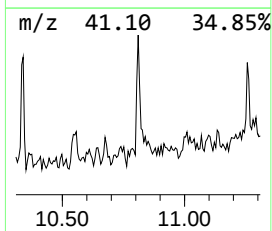
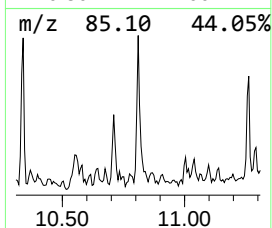
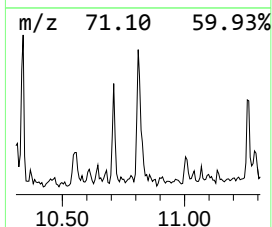
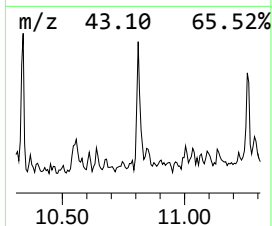
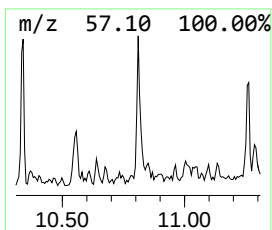
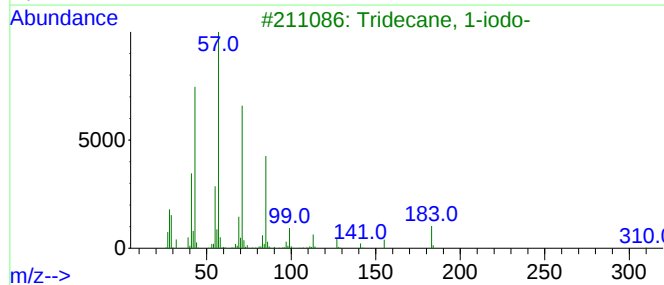
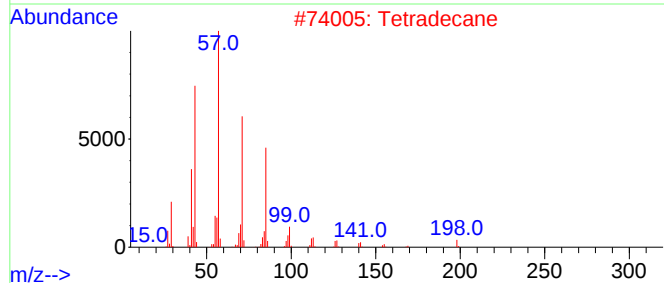
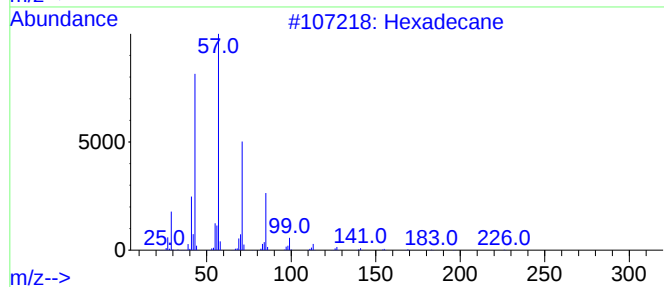
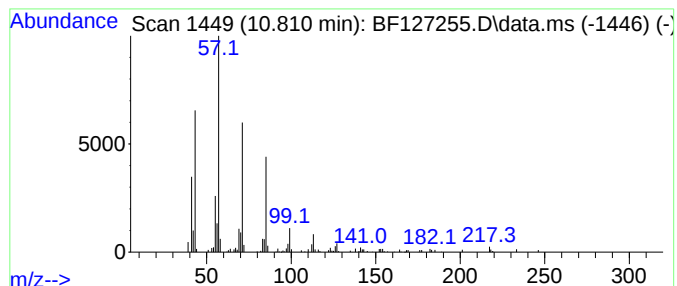
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Peak Number 4 Tetradecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.810	2.43 ng	75659	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	90
2			Tetradecane	198	C14H30	000629-59-4	90
3			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
4			Heptadecane	240	C17H36	000629-78-7	86
5			Nonadecane	268	C19H40	000629-92-5	83



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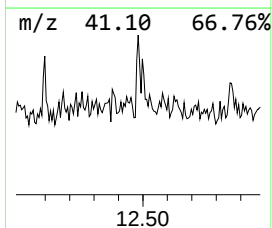
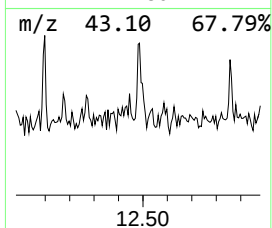
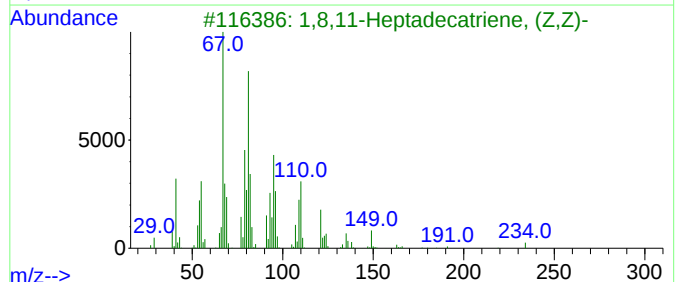
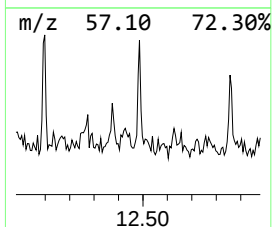
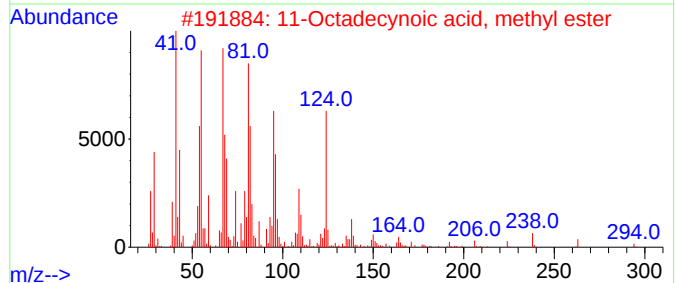
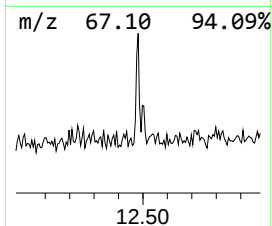
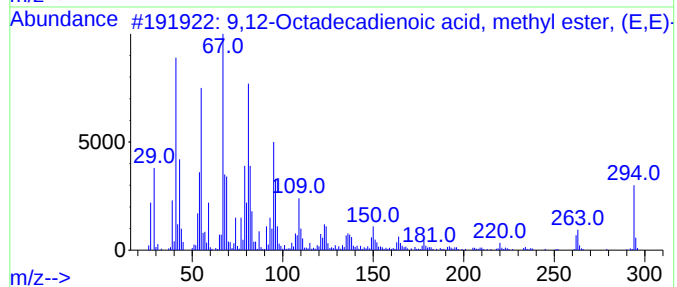
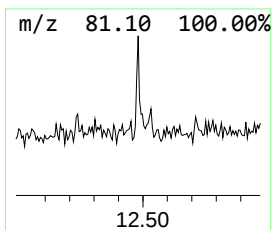
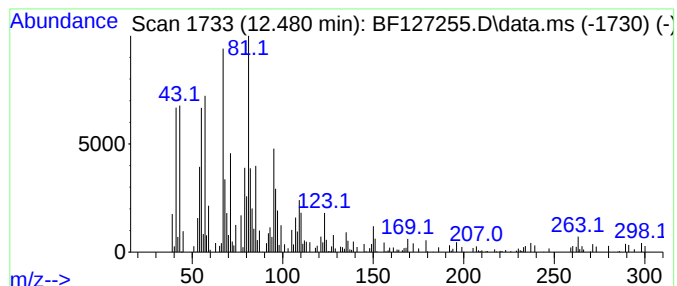
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.480	2.24 ng	69692	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	93		
2	11-Octadecynoic acid, methyl ester	294	C19H34O2	026543-37-3	89		
3	1,8,11-Heptadecatriene, (Z,Z)-	234	C17H30	056134-03-3	83		
4	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	83		
5	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	78		



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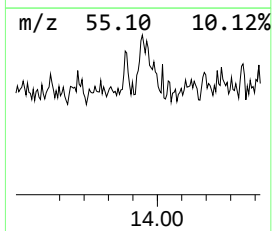
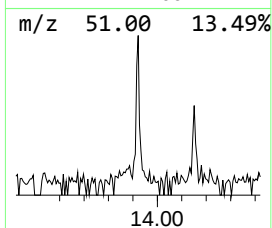
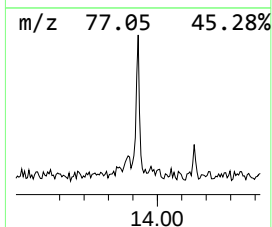
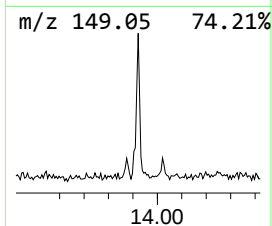
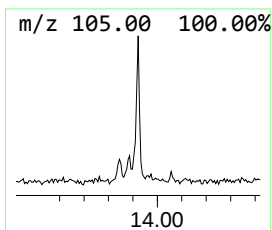
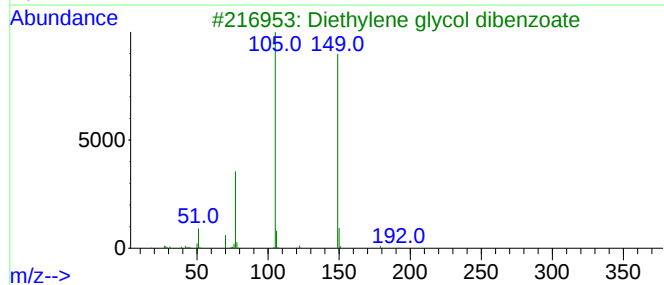
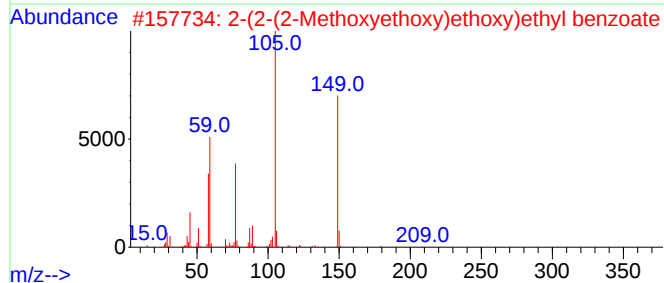
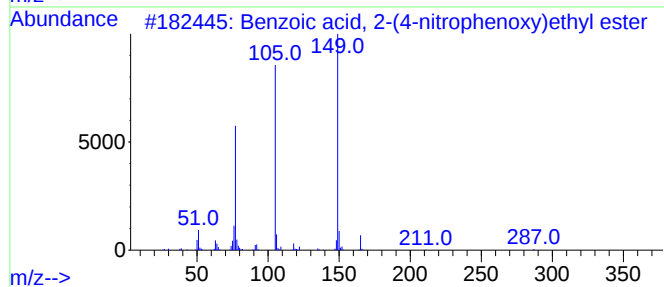
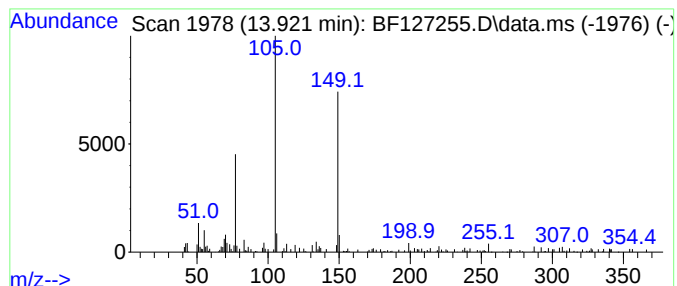
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzoic acid, 2-(4-nitrophe... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	5.87 ng	101545	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	72
2			2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	72
3			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	59
4			3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	59
5			3H,4H-3-Methylpyrro(1,2-D)(1,2,4...	149	C7H7N3O	1000434-18-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030822\
Data File : BF127255.D
Acq On : 08 Mar 2022 13:34
Operator : CG\JU
Sample : N1763-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
23-24-SAMPLE-LOCATION-12

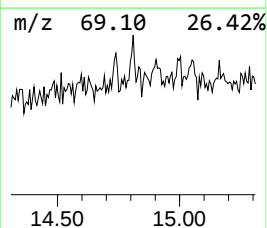
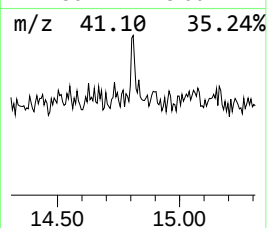
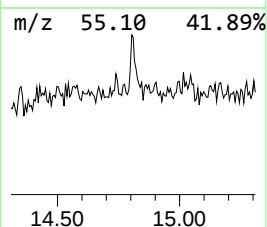
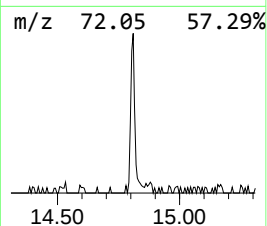
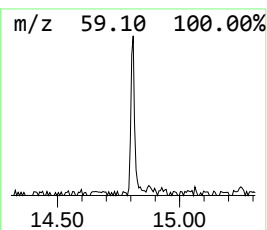
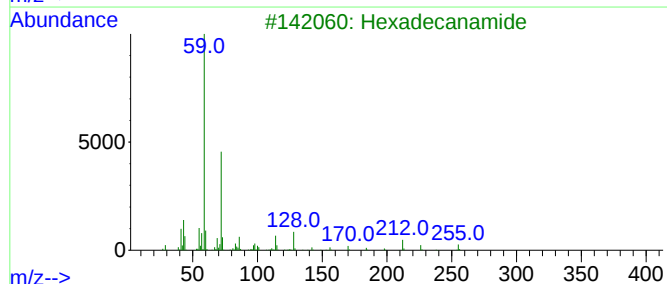
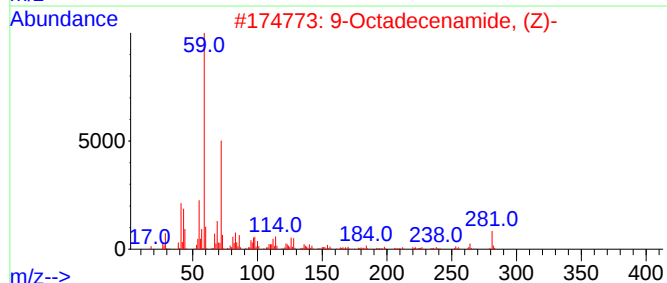
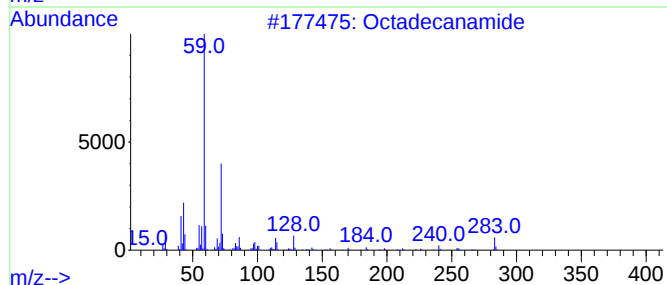
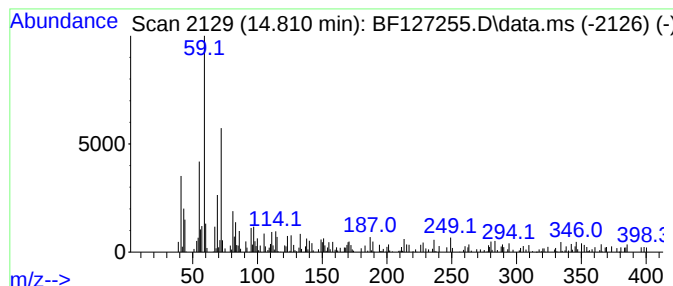
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanamide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.810	3.34 ng	70507	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanamide	283	C18H37NO	000124-26-5	74
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	74
3			Hexadecanamide	255	C16H33NO	000629-54-9	64
4			Nonadecanamide	297	C19H39NO	058185-32-3	64
5			N-Chloroacetyl-dl-erythro-0-meth...	209	C7H12ClNO4	1010214-48-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030822\
Data File : BF127255.D
Acq On : 08 Mar 2022 13:34
Operator : CG\JU
Sample : N1763-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
23-24-SAMPLE-LOCATION-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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
Decane, 3,6-dim...	9.304	2.1	ng	74602	3	9.922	705256	20.0
Heptadecane	9.833	2.1	ng	72846	3	9.922	705256	20.0
Hexadecane	10.339	2.0	ng	71692	3	9.922	705256	20.0
Tetradecane	10.810	2.4	ng	75659	4	11.410	621465	20.0
9,12-Octadecadi...	12.480	2.2	ng	69692	4	11.410	621465	20.0
unknown13.874	13.874	3.7	ng	63815	5	14.057	345762	20.0
Benzoic acid, 2...	13.921	5.9	ng	101545	5	14.057	345762	20.0
Octadecanamide	14.810	3.3	ng	70507	6	15.551	422104	20.0