

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
 Data File : BF117557.D
 Acq On : 28 Oct 2019 13:23
 Operator : JU
 Sample : K5502-07
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 180-34-(0-2.1)

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BF101819.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.351	551	555	580	rBV	543425	757308	84.43%	9.412%
2	6.381	726	730	747	rBV	793972	878435	97.93%	10.917%
3	6.504	747	751	767	rVB	908174	897012	100.00%	11.148%
4	6.728	785	789	796	rBV	233281	235455	26.25%	2.926%
5	6.881	811	815	829	rBV	685892	610160	68.02%	7.583%
6	7.292	881	885	906	rBV	462236	522421	58.24%	6.493%
7	8.010	1003	1007	1024	rBV	277945	315243	35.14%	3.918%
8	9.080	1185	1189	1203	rBV	957434	851290	94.90%	10.580%
9	9.480	1253	1257	1267	rBB	88693	88789	9.90%	1.103%
10	9.757	1301	1304	1318	rBV	382925	359424	40.07%	4.467%
11	10.551	1436	1439	1452	rBV	504281	528735	58.94%	6.571%
12	11.245	1554	1557	1567	rBV	343872	358635	39.98%	4.457%
13	11.774	1643	1647	1655	rBV	34990	38987	4.35%	0.485%
14	12.468	1761	1765	1771	rBV	24497	23051	2.57%	0.286%
15	12.557	1775	1780	1787	rBV2	8104	11797	1.32%	0.147%
16	12.698	1798	1804	1811	rVB	19694	23984	2.67%	0.298%
17	12.827	1822	1826	1834	rBV	854533	741393	82.65%	9.214%
18	13.727	1972	1979	1990	rBV5	39220	72156	8.04%	0.897%
19	13.892	2003	2007	2016	rVB	257692	266556	29.72%	3.313%
20	14.039	2027	2032	2035	rBV2	15568	15865	1.77%	0.197%
21	14.345	2079	2084	2092	rBV	27755	32524	3.63%	0.404%
22	14.639	2130	2134	2139	rBV	43488	44198	4.93%	0.549%
23	14.709	2143	2146	2149	rVB	30753	29744	3.32%	0.370%
24	14.957	2185	2188	2192	rVB	50137	53044	5.91%	0.659%
25	15.327	2244	2251	2260	rVB	143588	233384	26.02%	2.901%
26	15.715	2312	2317	2321	rBV3	26248	38490	4.29%	0.478%
27	16.180	2392	2396	2400	rBV3	12175	18219	2.03%	0.226%

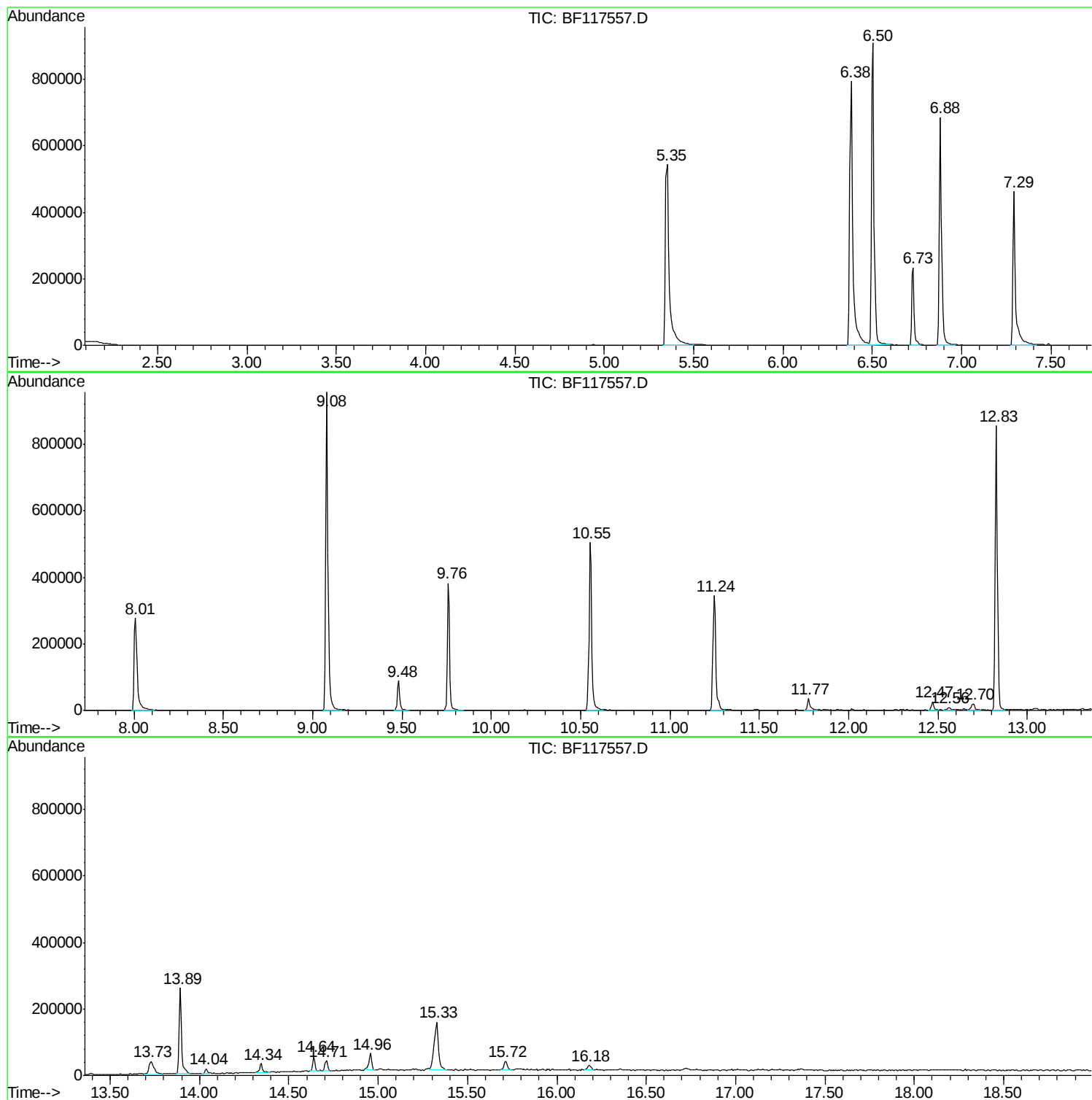
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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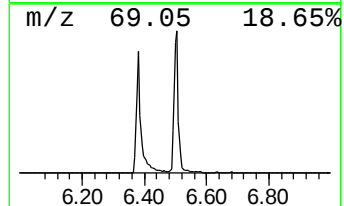
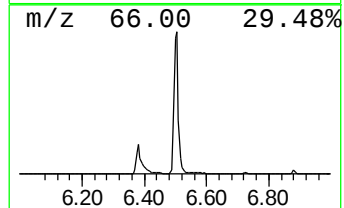
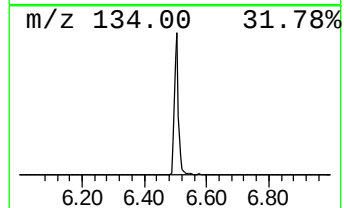
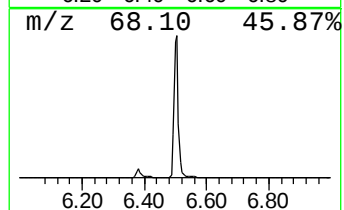
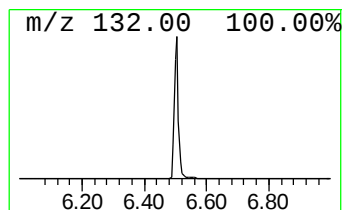
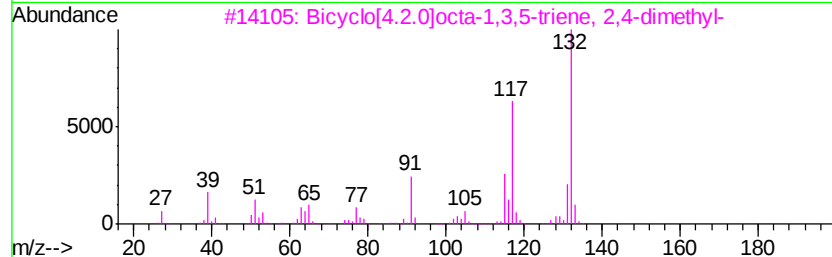
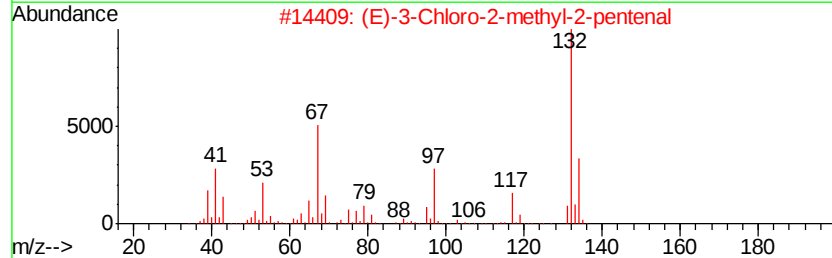
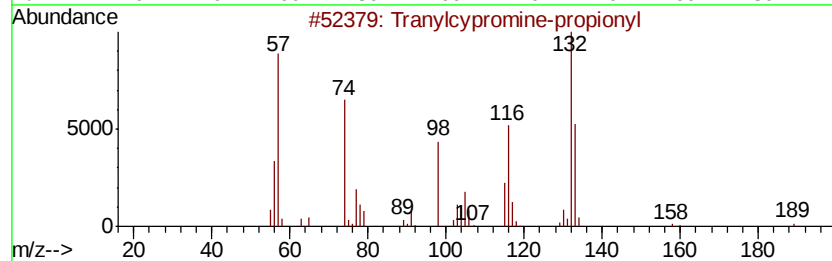
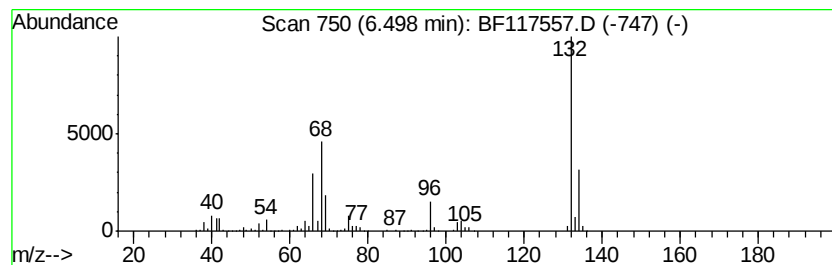
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	76.19 ng	897012	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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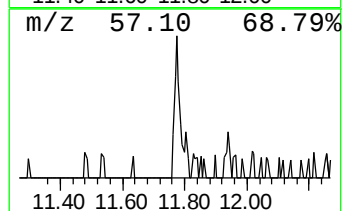
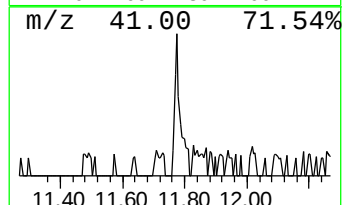
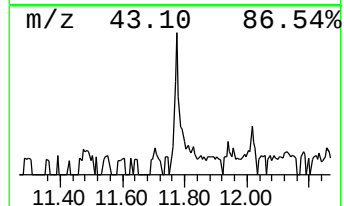
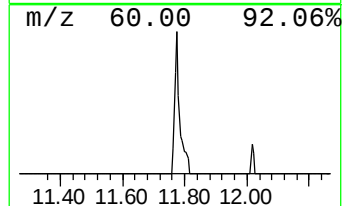
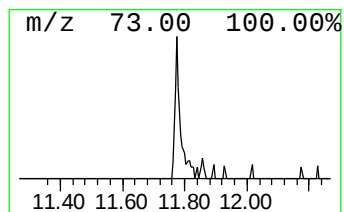
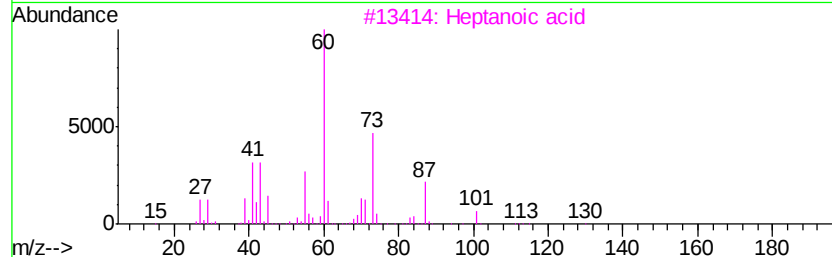
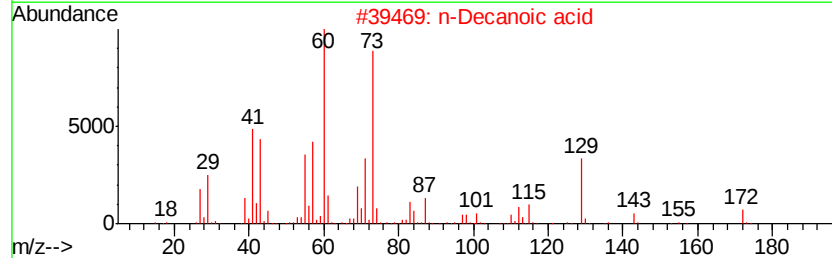
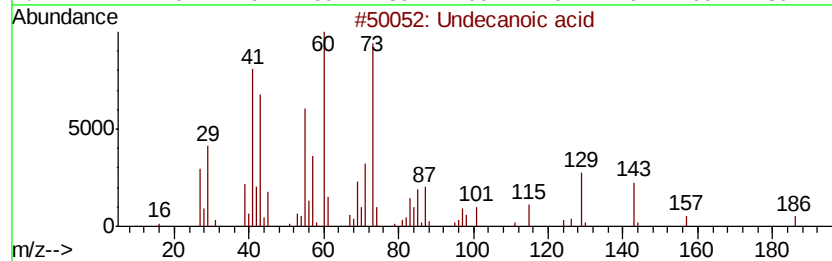
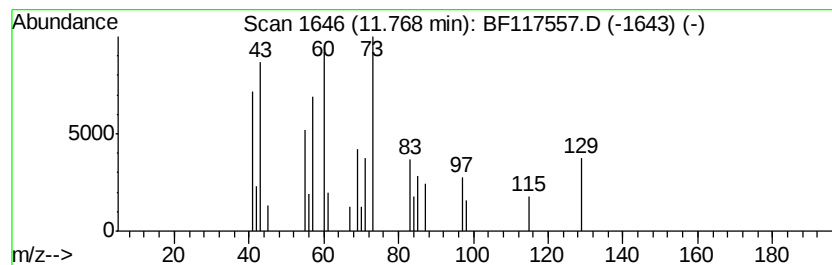
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Peak Number 3 Undecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	2.17 ng	38987	Phenanthrene-d10	11.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecanoic acid	186	C11H22O2	000112-37-8	50
2		n-Decanoic acid	172	C10H20O2	000334-48-5	50
3		Heptanoic acid	130	C7H14O2	000111-14-8	38
4		Trehalose	342	C12H22O11	000099-20-7	38
5		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38



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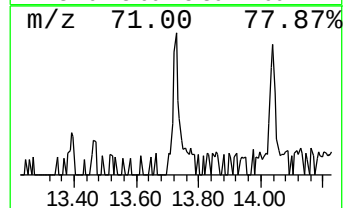
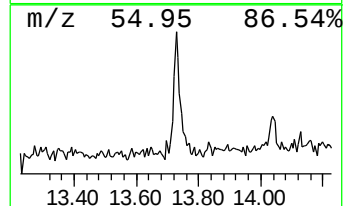
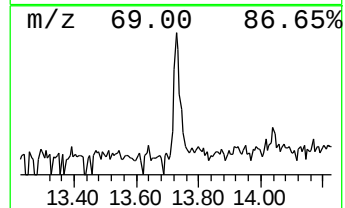
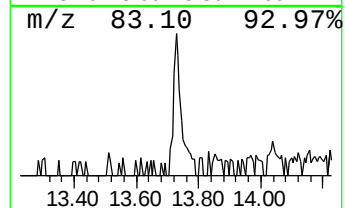
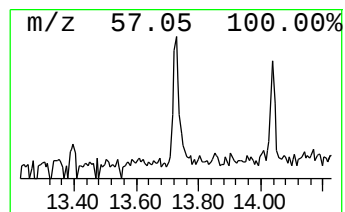
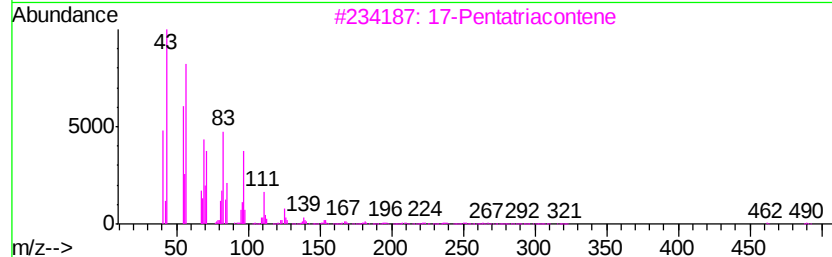
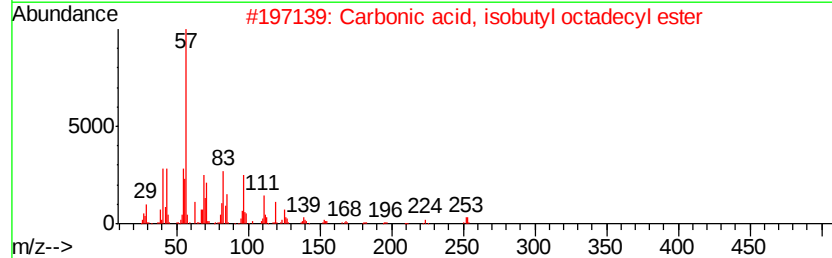
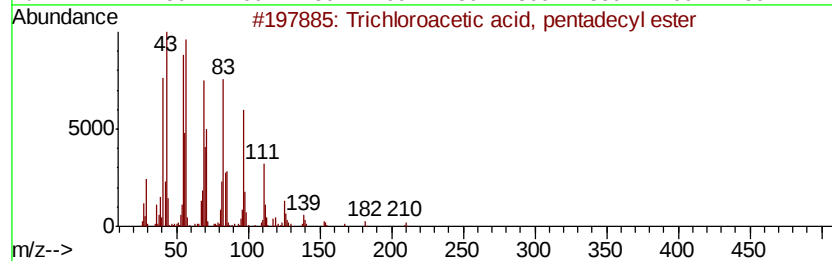
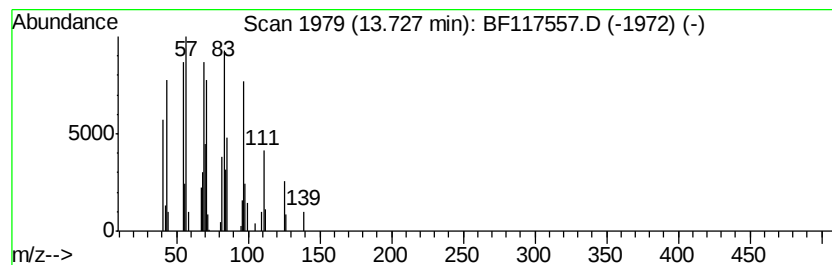
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Peak Number 4 Trichloroacetic acid, penta... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	5.41 ng	72156	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	74
2		Carbonic acid, isobutyl octadecyl...	370	C23H46O3	1000314-61-5	72
3		17-Pentatriacontene	491	C35H70	006971-40-0	72
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	72
5		Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	72



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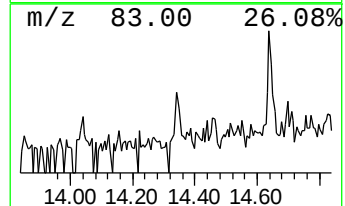
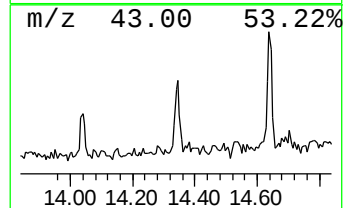
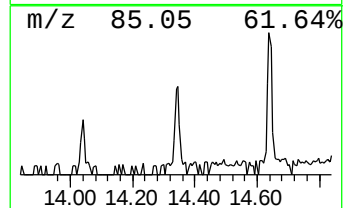
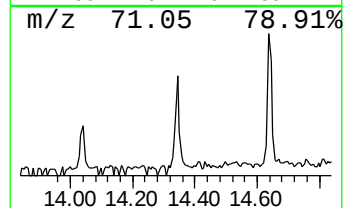
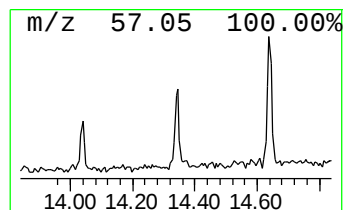
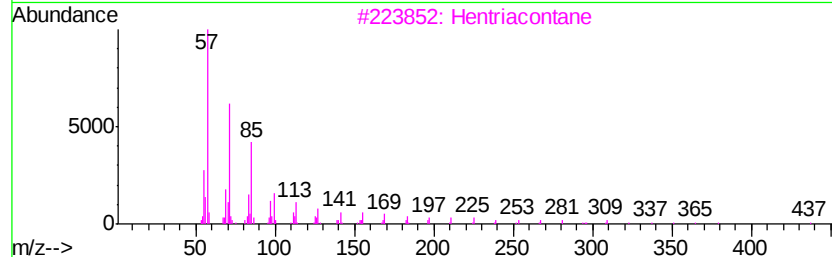
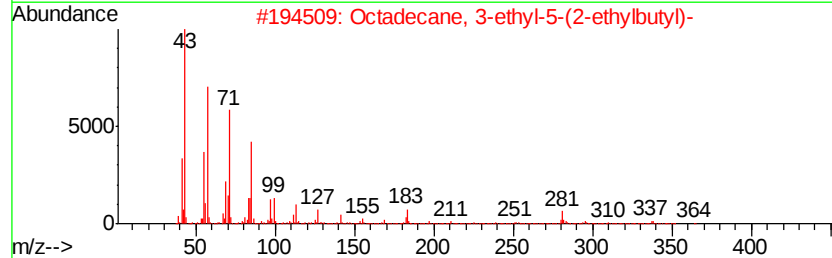
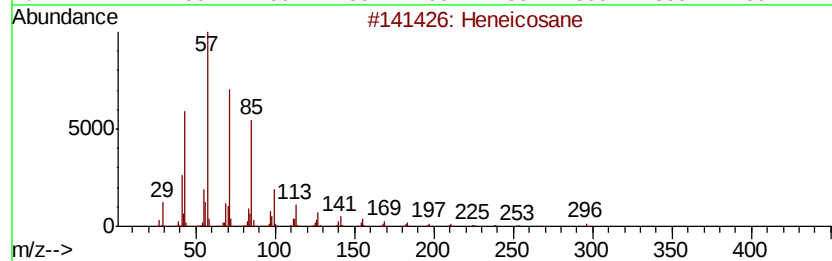
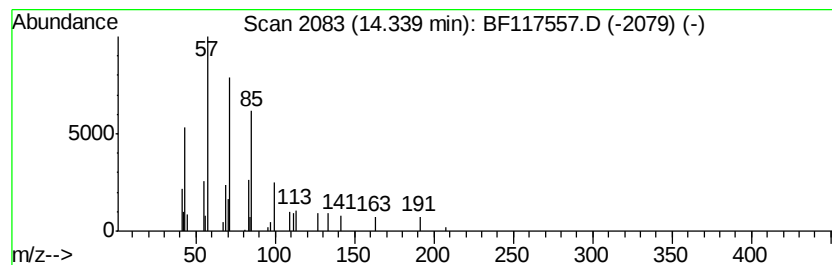
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Peak Number 5 Octadecane, 3-ethyl-5-(2-ethylbu... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.34	2.44 ng	32524	Chrysene-d12		13.89
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	86
3	Hentriacontane	437	C31H64	000630-04-6	86
4	Hexatriacontane	507	C36H74	000630-06-8	83
5	Hexadecane	226	C16H34	000544-76-3	80



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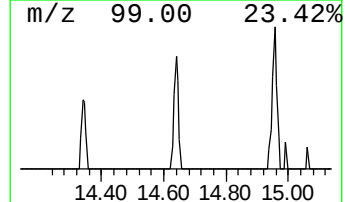
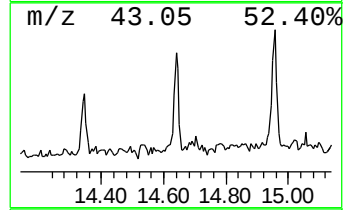
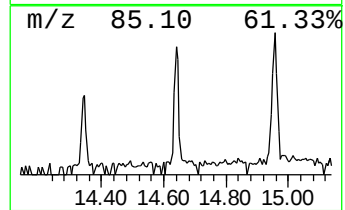
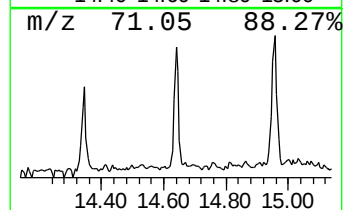
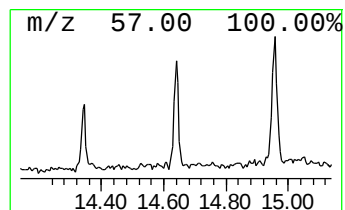
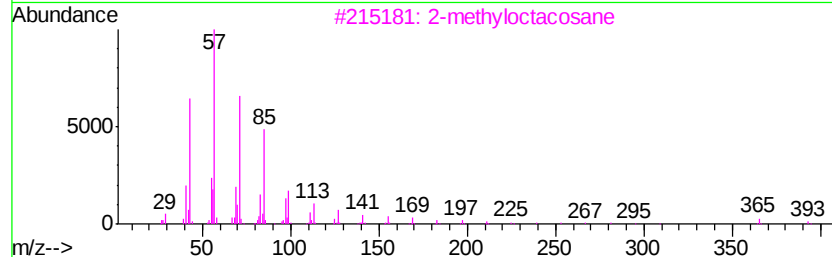
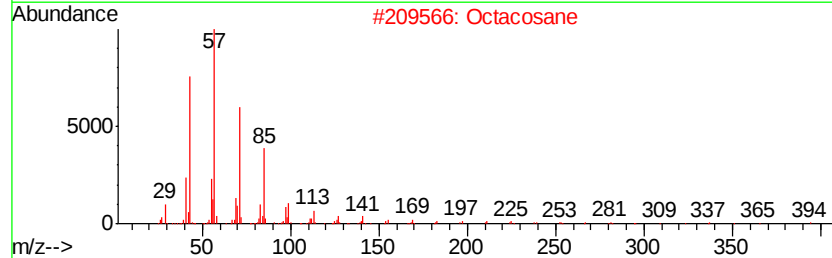
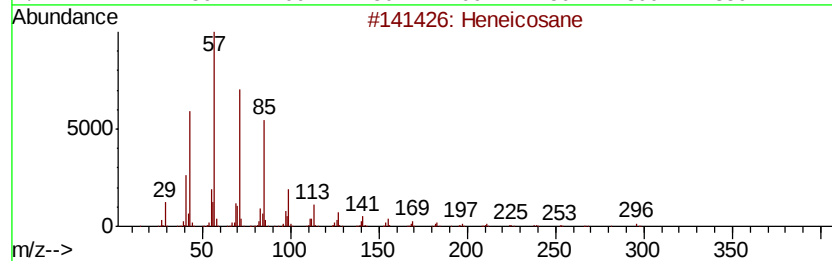
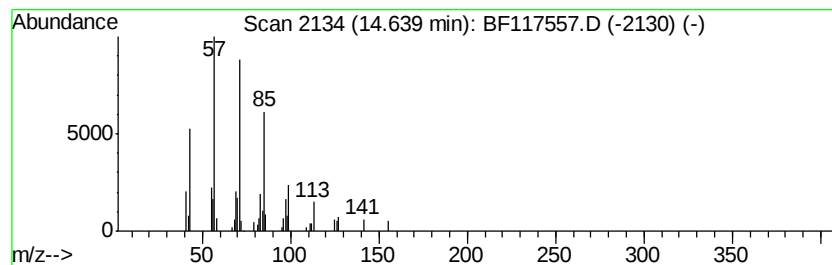
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	3.79 ng	44198	Perylene-d12	15.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Octacosane		394	C28H58	000630-02-4	87
3	2-methyloctacosane		408	C29H60	1000376-72-8	83
4	Heptacosane		380	C27H56	000593-49-7	83
5	Hexacosane		366	C26H54	000630-01-3	80



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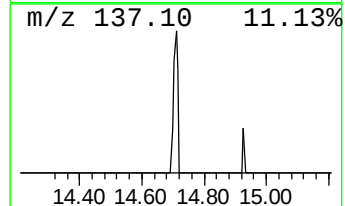
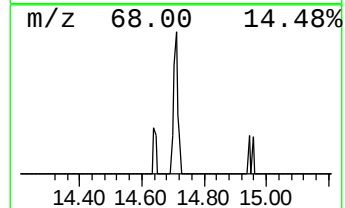
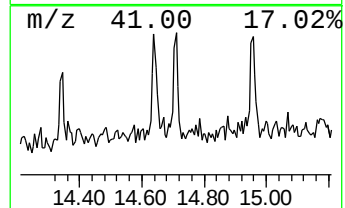
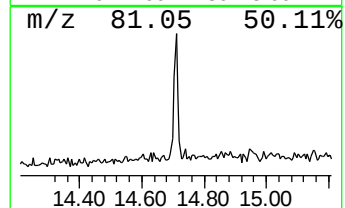
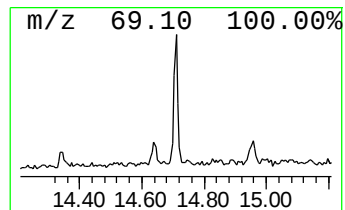
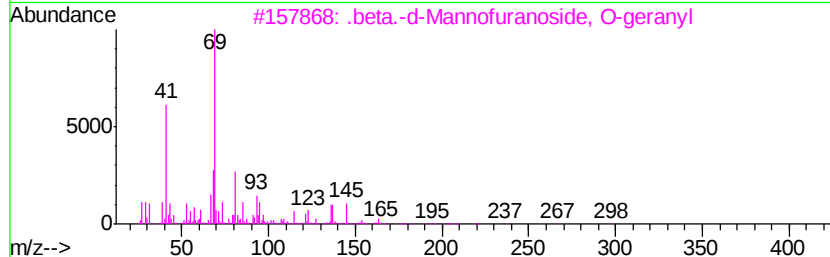
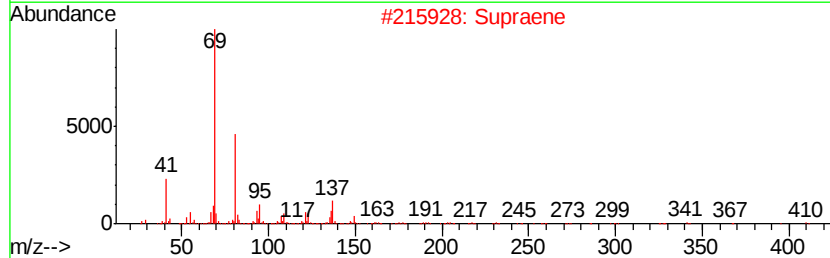
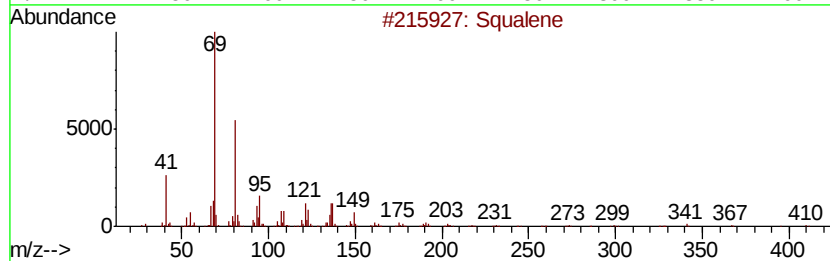
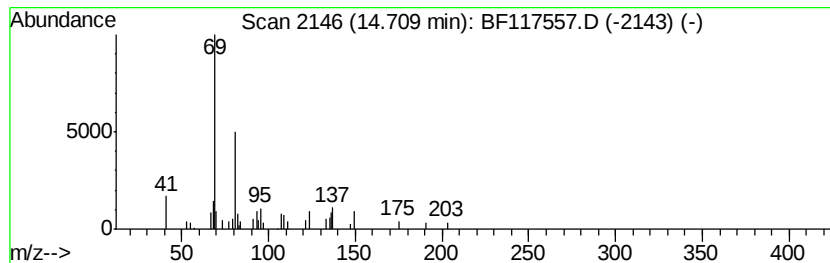
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	2.55 ng	29744	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	86
2		Supraene	410	C30H50	007683-64-9	80
3		.beta.-d-Mannofuranoside, O-geranyl	316	C16H28O6	1000154-77-2	64
4		2,6,10-Dodecatrienal, 3,7,11-tri...	220	C15H24O	000502-67-0	64
5		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117557.D
Acq On : 28 Oct 2019 13:23
Operator : JU
Sample : K5502-07
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
180-34-(0-2.1)

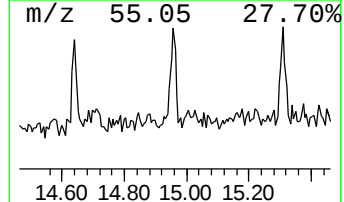
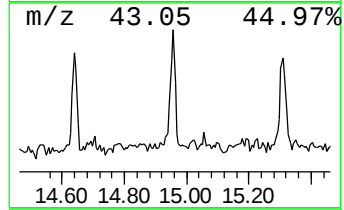
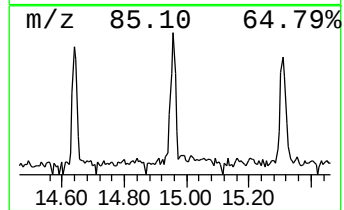
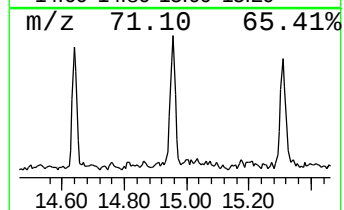
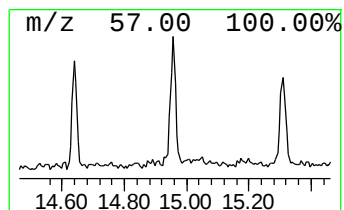
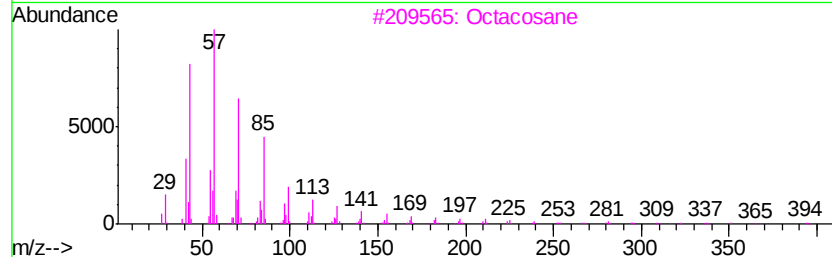
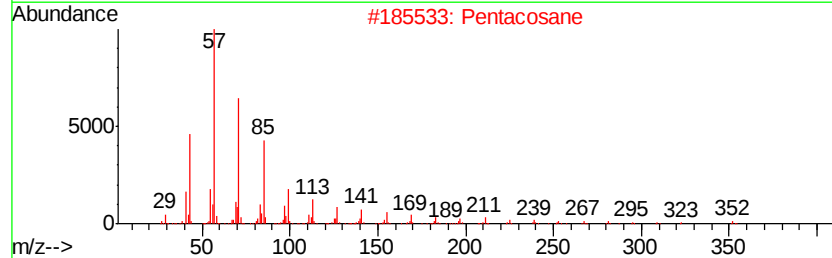
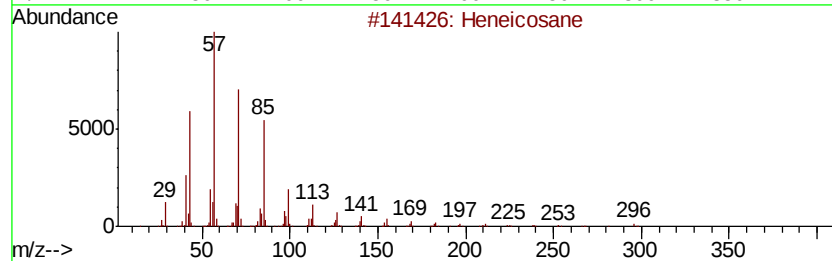
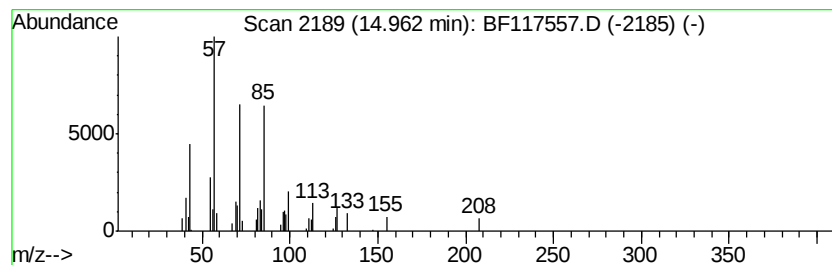
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Pentacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	4.55 ng	53044	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Pentacosane	352	C25H52	000629-99-2	91
3		Octacosane	394	C28H58	000630-02-4	91
4		triacontane	422	C30H62	000638-68-6	91
5		Heptadecane	240	C17H36	000629-78-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117557.D
Acq On : 28 Oct 2019 13:23
Operator : JU
Sample : K5502-07
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
180-34-(0-2.1)

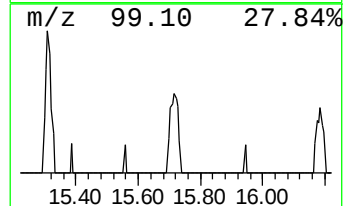
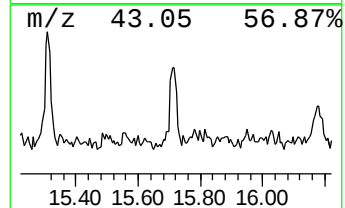
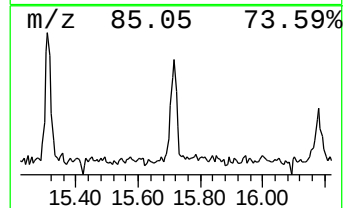
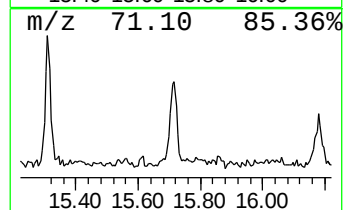
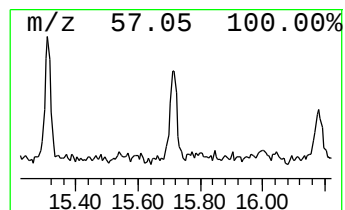
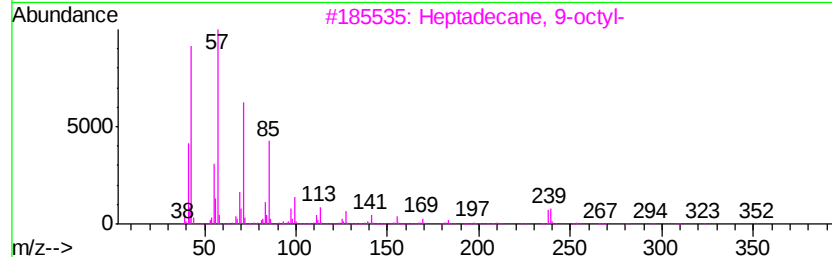
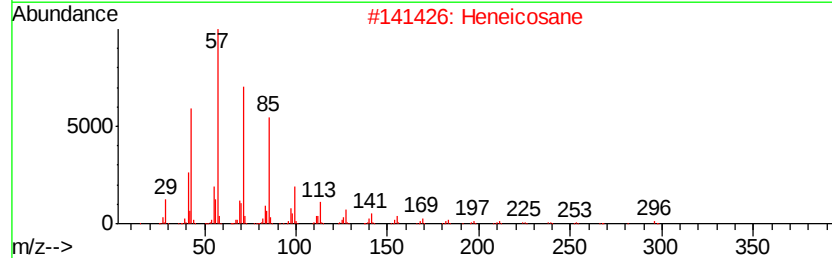
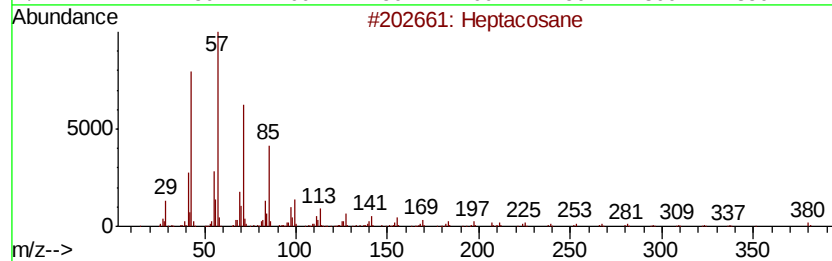
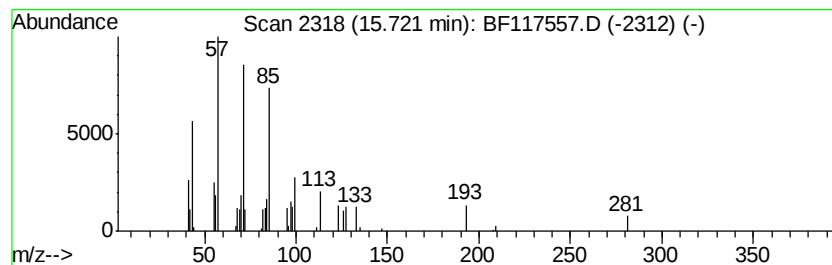
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	3.30 ng	38490	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	91
2		Heneicosane	296	C21H44	000629-94-7	87
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
4		Octadecane	254	C18H38	000593-45-3	80
5		Nonadecane	268	C19H40	000629-92-5	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102819\
Data File : BF117557.D
Acq On : 28 Oct 2019 13:23
Operator : JU
Sample : K5502-07
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
180-34-(0-2.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.50	6.50	76.2	ng	897012	1	6.73	235455	20.0
Undecanoic acid	11.77	2.2	ng	38987	4	11.24	358635	20.0
Trichloroacetic a...	13.73	5.4	ng	72156	5	13.89	266556	20.0
Octadecane, 3-eth...	14.34	2.4	ng	32524	5	13.89	266556	20.0
Heneicosane	14.64	3.8	ng	44198	6	15.33	233384	20.0
Squalene	14.71	2.5	ng	29744	6	15.33	233384	20.0
Pentacosane	14.96	4.5	ng	53044	6	15.33	233384	20.0
Heptacosane	15.72	3.3	ng	38490	6	15.33	233384	20.0