

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082519\
 Data File : BF116531.D
 Acq On : 25 Aug 2019 14:53
 Operator : HP/JU
 Sample : K4493-10
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 T9-12-13-K1-K4-(0-1.9)

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-BF082319.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	2.246	19	27	33	rVB	2033748	2759888	81.71%	8.430%
2	3.451	225	232	240	rBV2	31513	54284	1.61%	0.166%
3	4.798	454	461	468	rVB	29918	41599	1.23%	0.127%
4	5.510	576	582	585	rBV	2858214	2904920	86.00%	8.873%
5	6.510	746	752	755	rBV	2754827	3185446	94.31%	9.730%
6	6.657	771	777	780	rBV	3207406	3179610	94.14%	9.712%
7	6.881	812	815	819	rBV	985871	886802	26.25%	2.709%
8	7.039	838	842	846	rBV	2497911	2439886	72.24%	7.453%
9	7.439	904	910	913	rBV	1879896	2000835	59.24%	6.112%
10	8.163	1028	1033	1036	rBV	1343064	1161122	34.38%	3.547%
11	8.239	1042	1046	1052	rVB2	43505	48126	1.42%	0.147%
12	8.763	1131	1135	1140	rVB2	68987	57900	1.71%	0.177%
13	8.875	1148	1154	1157	rBV	47385	38430	1.14%	0.117%
14	8.910	1157	1160	1167	rVB	43729	44769	1.33%	0.137%
15	9.239	1210	1216	1219	rBV	4004412	3377663	100.00%	10.317%
16	9.622	1279	1281	1287	rVB	267596	230891	6.84%	0.705%
17	9.916	1325	1331	1334	rBV	1553908	1236378	36.60%	3.777%
18	10.622	1447	1451	1455	rBV	55983	55792	1.65%	0.170%
19	10.698	1460	1464	1468	rBV	1716312	1498864	44.38%	4.578%
20	11.398	1579	1583	1585	rBV	1273695	1082926	32.06%	3.308%
21	11.422	1585	1587	1589	rVV	308687	230894	6.84%	0.705%
22	11.469	1589	1595	1597	rVV3	78515	114297	3.38%	0.349%
23	11.921	1670	1672	1675	rBV2	190175	180073	5.33%	0.550%
24	12.610	1786	1789	1791	rVB	392959	330932	9.80%	1.011%
25	12.833	1825	1827	1831	rVB	251133	227797	6.74%	0.696%
26	12.980	1848	1852	1856	rBV	2289814	2246299	66.50%	6.862%
27	13.880	2002	2005	2010	rVB2	219934	232211	6.87%	0.709%
28	14.033	2026	2031	2033	rBV2	762198	872923	25.84%	2.666%
29	14.057	2033	2035	2040	rVB	142106	127189	3.77%	0.389%
30	15.068	2204	2207	2215	rVB	157768	300471	8.90%	0.918%
31	15.157	2219	2222	2231	rVB2	166225	259609	7.69%	0.793%
32	15.368	2256	2258	2264	rVB	85233	107266	3.18%	0.328%
33	15.427	2266	2268	2275	rVV	117675	157249	4.66%	0.480%
34	15.498	2276	2280	2283	rVV	515700	618705	18.32%	1.890%

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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-BF082319.M
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35	15.539	2284	2287	2294	rVB2	165968	231379	6.85%	0.707%
36	15.980	2359	2362	2367	rVB	108697	144114	4.27%	0.440%
37	16.498	2446	2450	2452	rBV	47724	70182	2.08%	0.214%

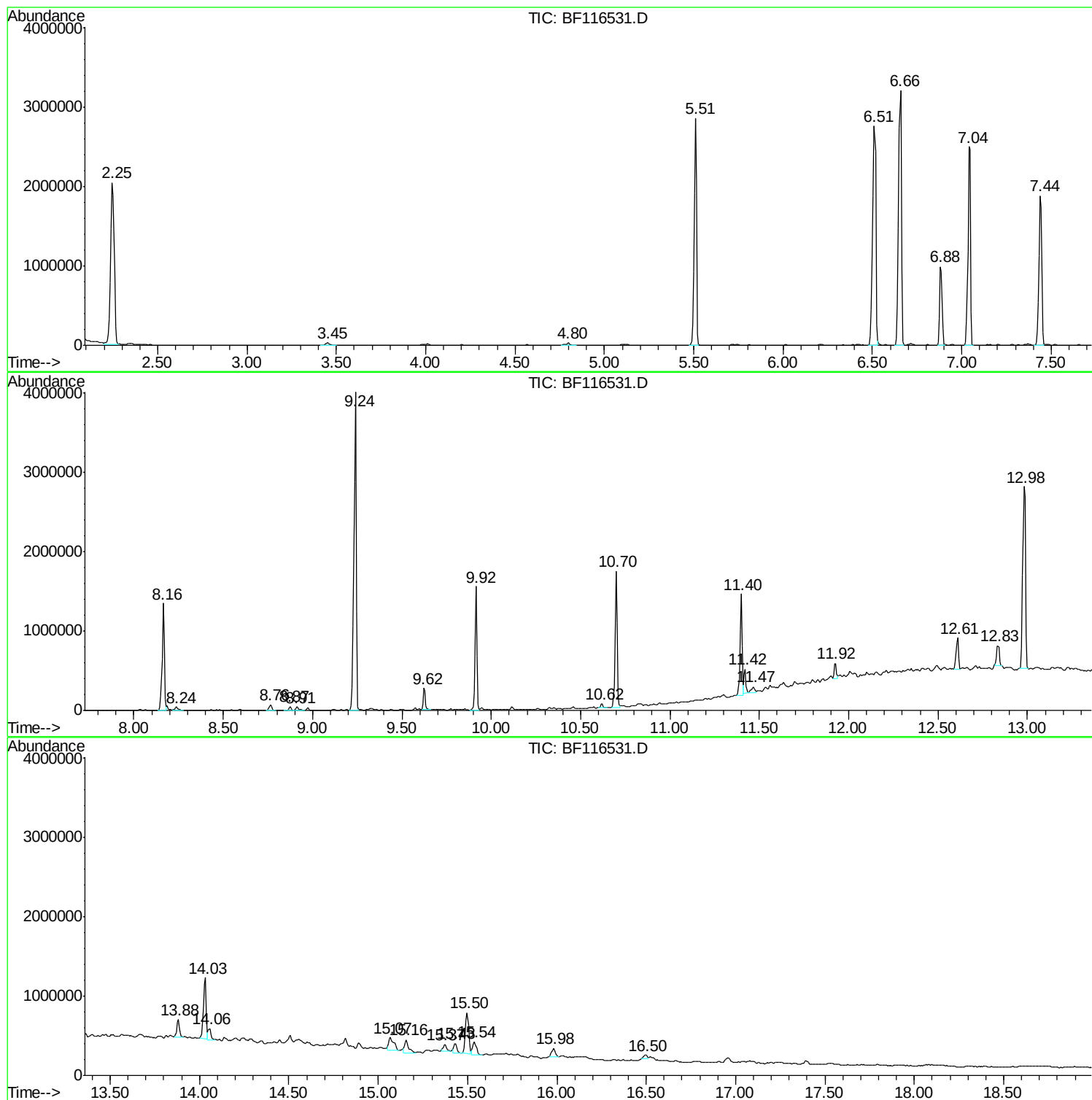
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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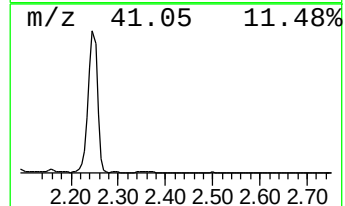
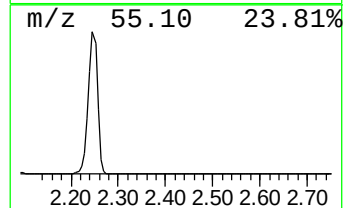
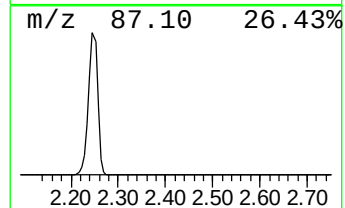
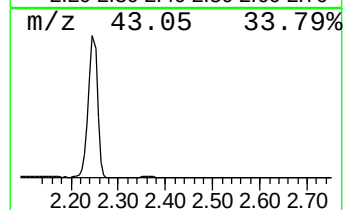
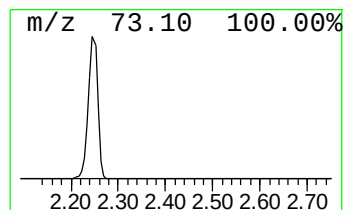
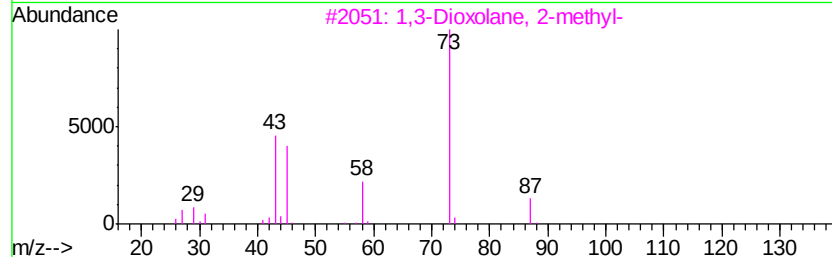
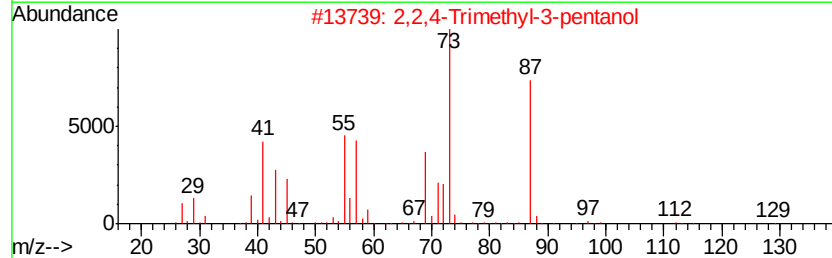
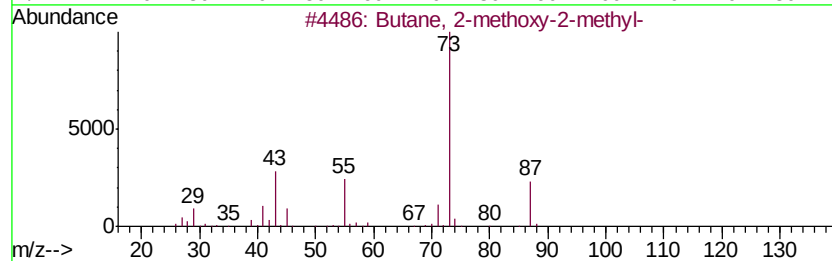
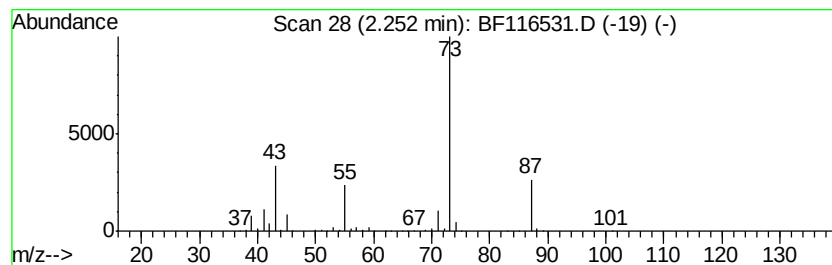
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	62.24 ng	2759890	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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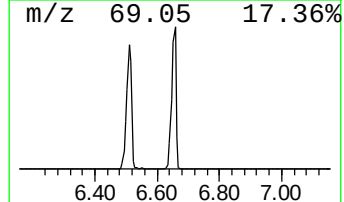
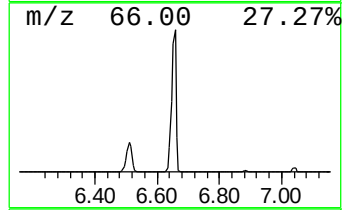
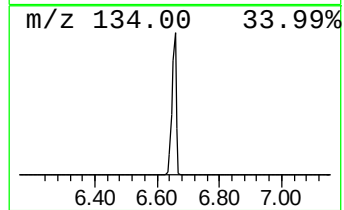
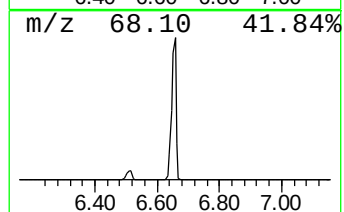
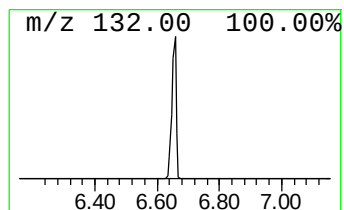
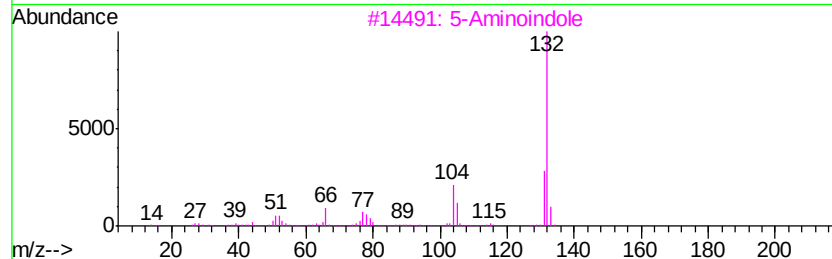
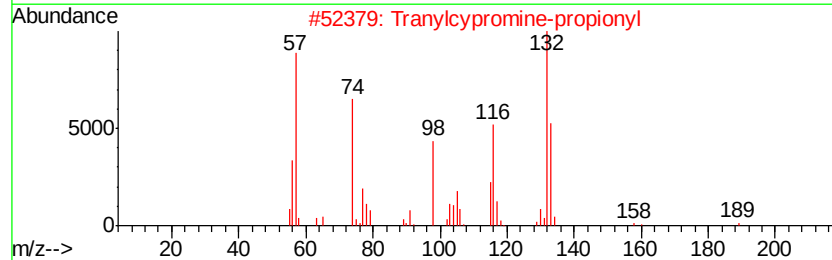
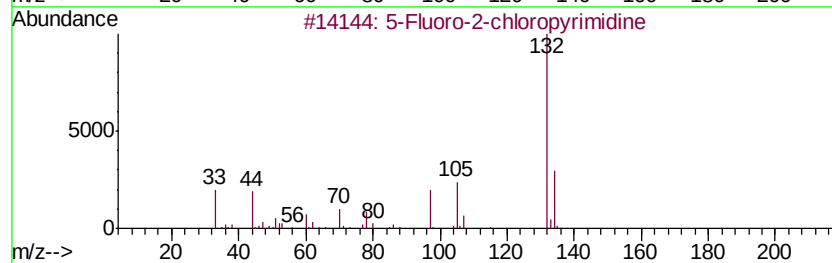
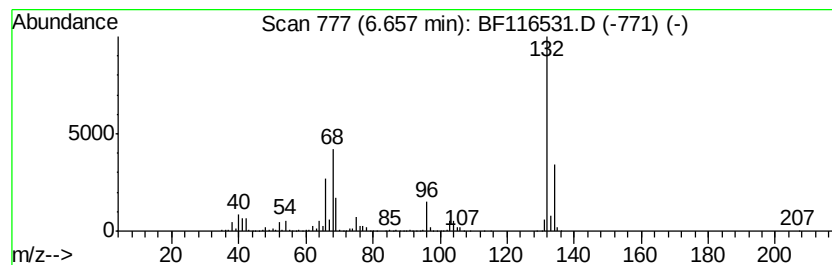
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF082319.M
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	71.71 ng	3179610	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3			5-Aminoindole	132	C8H8N2	005192-03-0	12
4			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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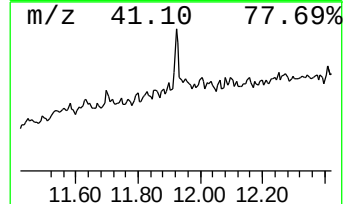
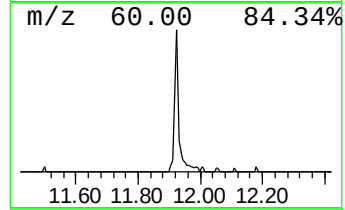
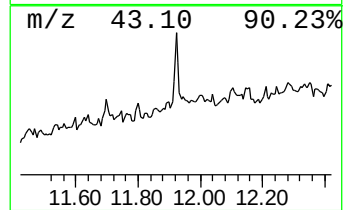
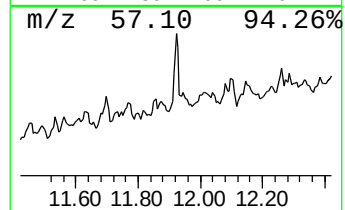
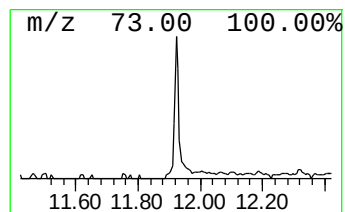
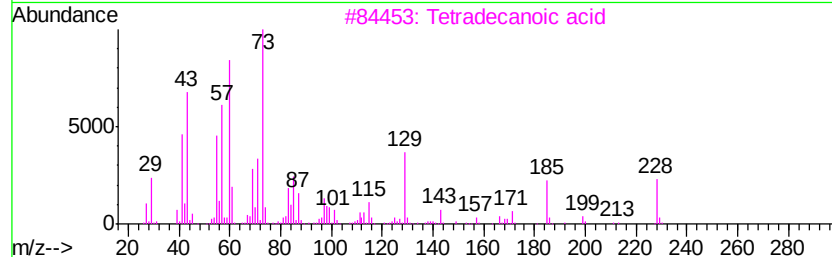
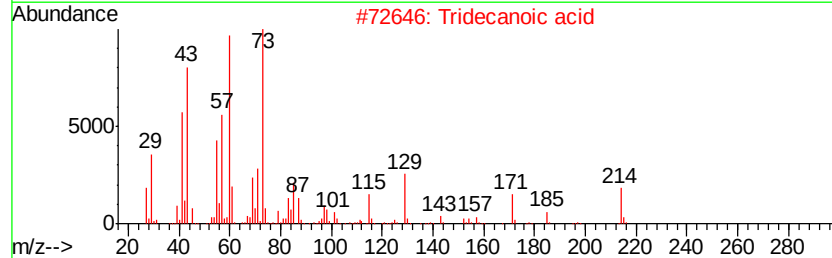
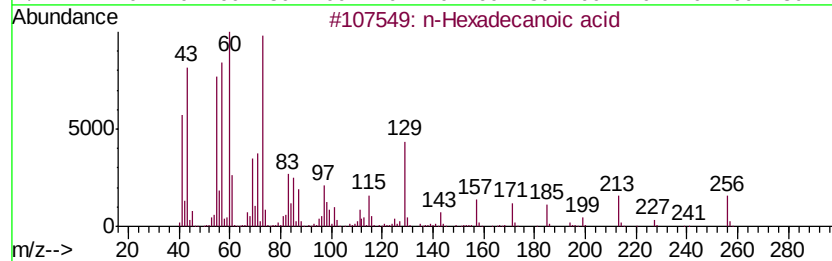
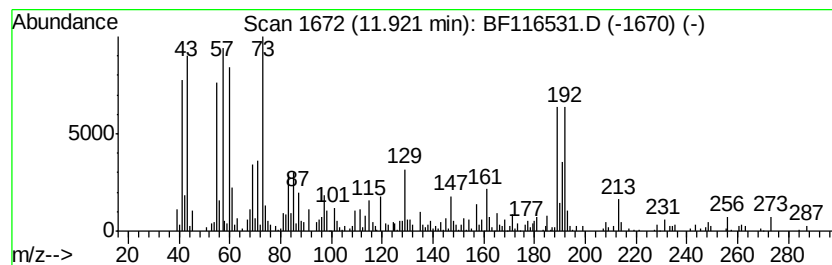
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.92	3.33 ng	180073	Phenanthrene-d10		11.40	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	97
2	Tridecanoic acid		214	C13H26O2	000638-53-9	78
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	78
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	53
5	Octadecanoic acid		284	C18H36O2	000057-11-4	49



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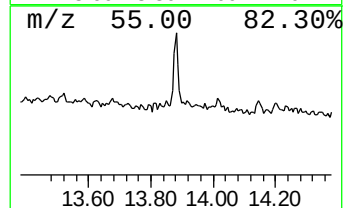
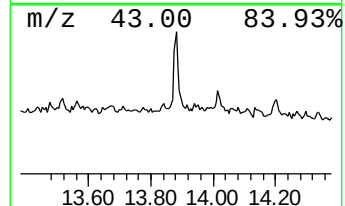
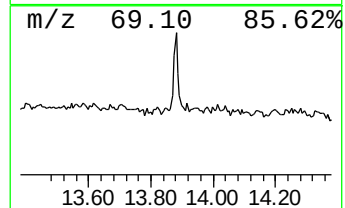
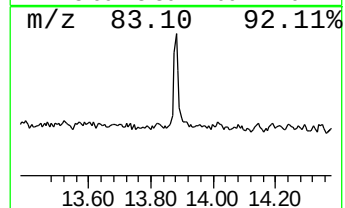
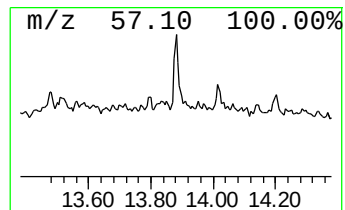
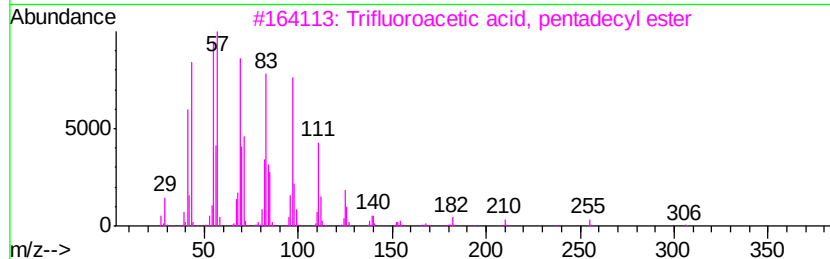
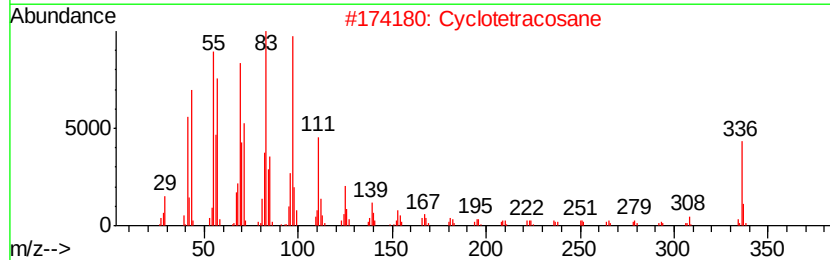
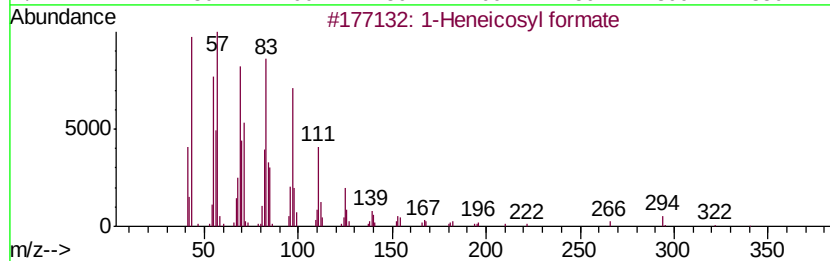
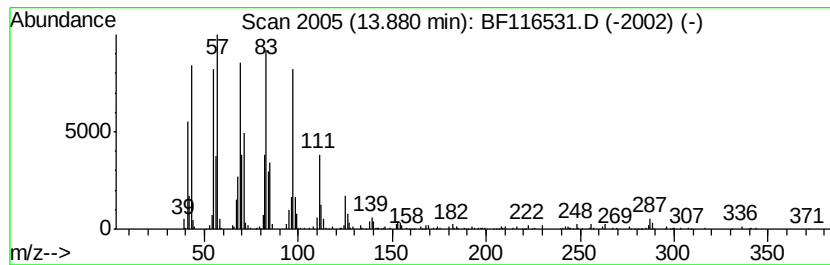
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Heneicosyl formate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.88	5.32 ng	232211	Chrysene-d12		14.03
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	99
2	Cyclotetracosane	336	C24H48	000297-03-0	95
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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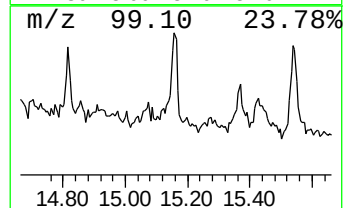
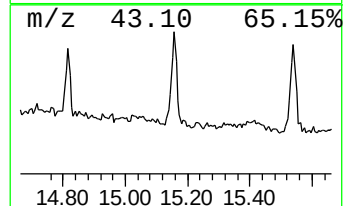
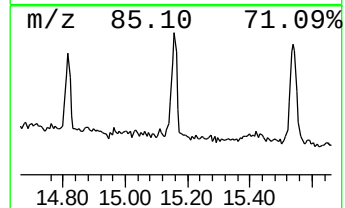
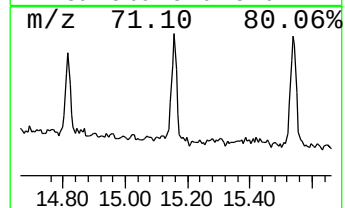
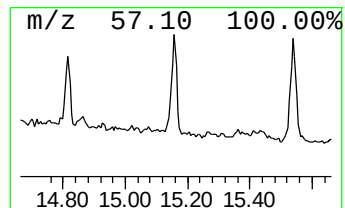
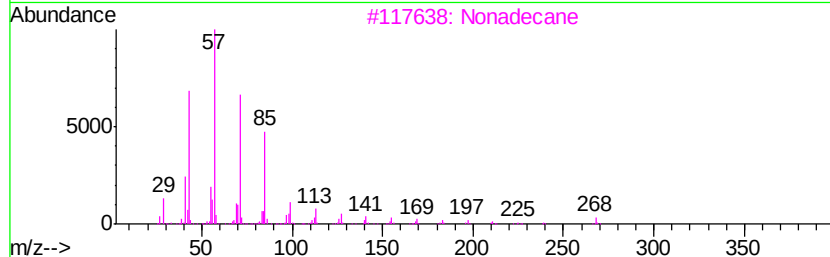
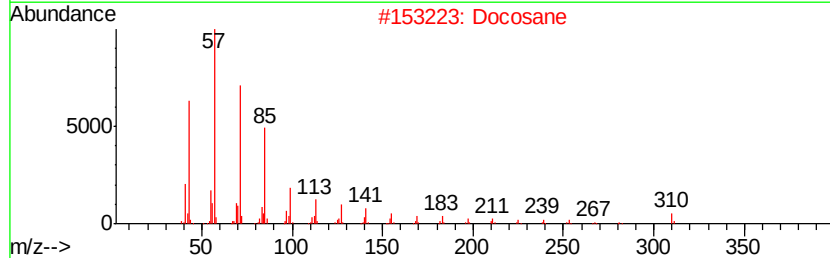
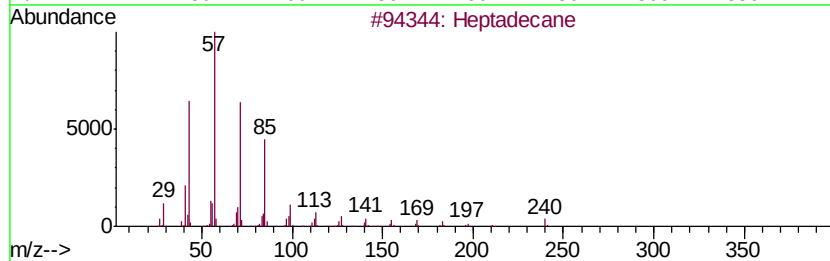
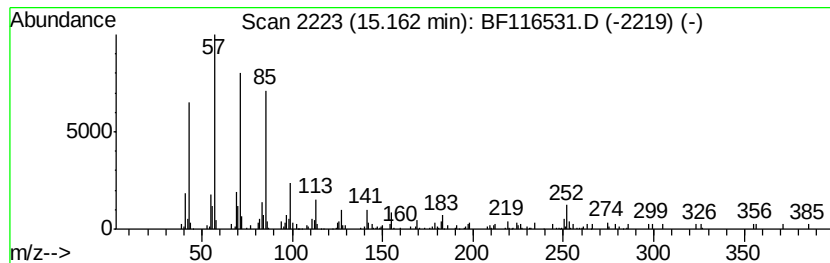
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	8.39 ng	259609	Perylene-d12	15.50
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	87
2	Docosane	310 C22H46	000629-97-0	87
3	Nonadecane	268 C19H40	000629-92-5	87
4	Octadecane, 1-iodo-	380 C18H37I	000629-93-6	87
5	Triacontane	422 C30H62	000638-68-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082519\
Data File : BF116531.D
Acq On : 25 Aug 2019 14:53
Operator : HP/JU
Sample : K4493-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T9-12-13-K1-K4-(0-1.9)

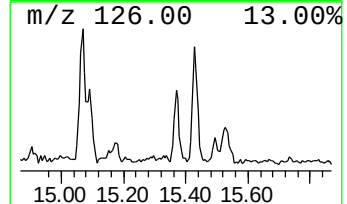
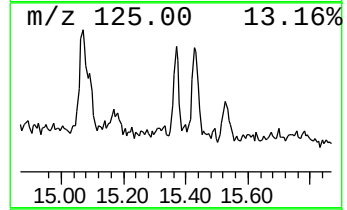
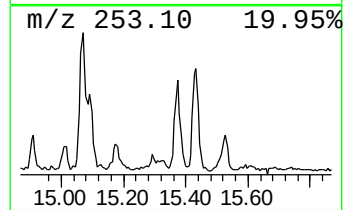
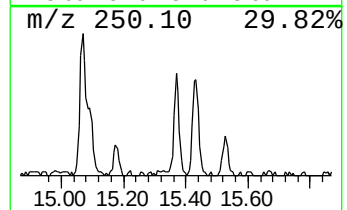
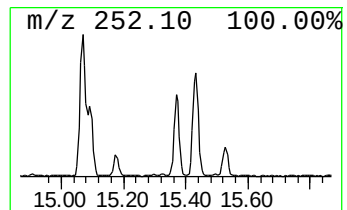
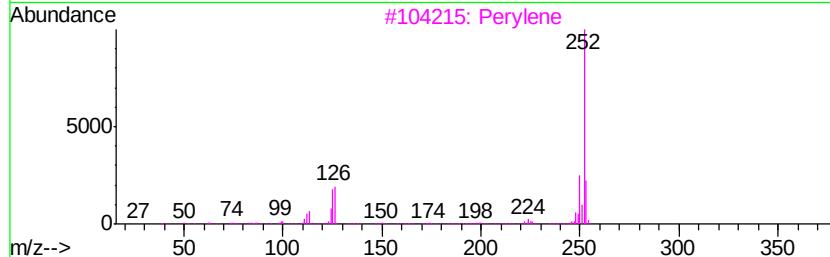
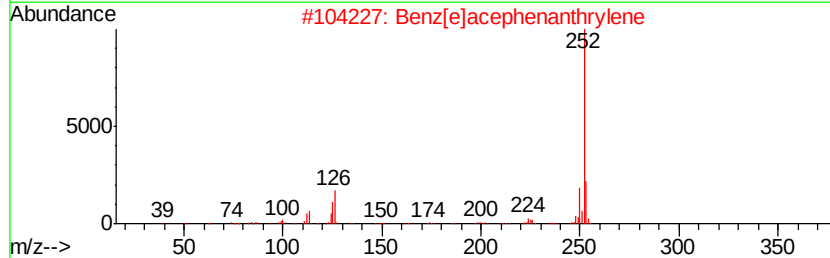
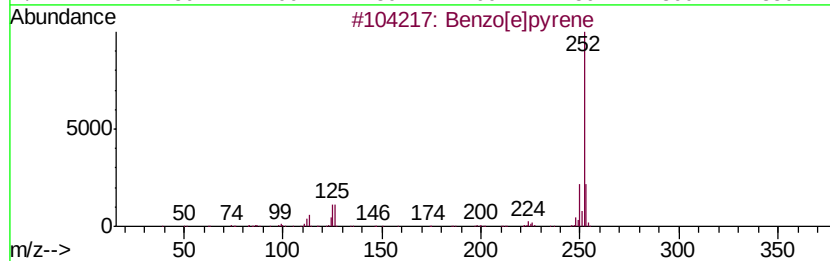
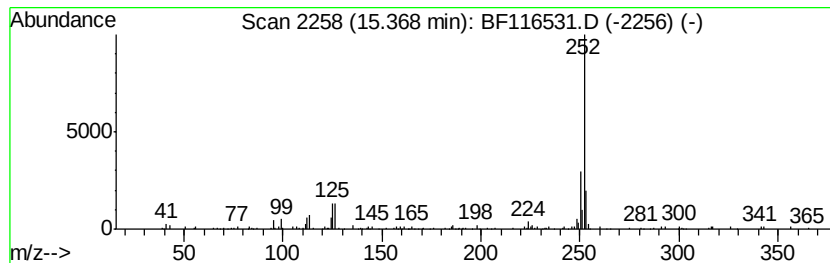
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	3.47 ng	107266	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94
3		Perylene	252	C20H12	000198-55-0	94
4		Benzo[a]pyrene	252	C20H12	000050-32-8	90
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082519\
Data File : BF116531.D
Acq On : 25 Aug 2019 14:53
Operator : HP/JU
Sample : K4493-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

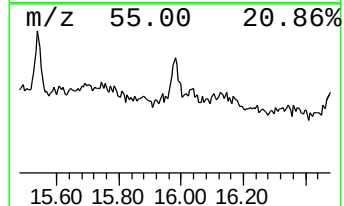
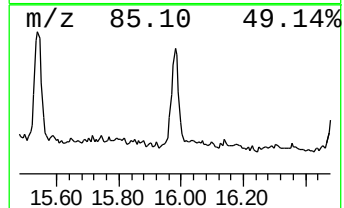
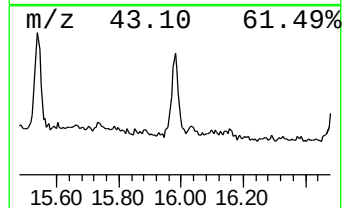
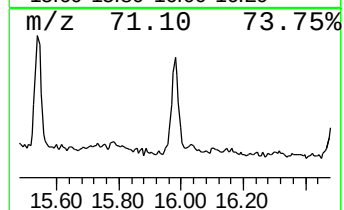
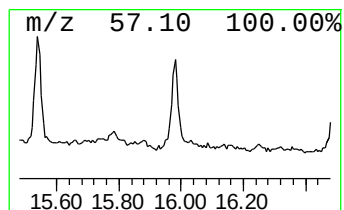
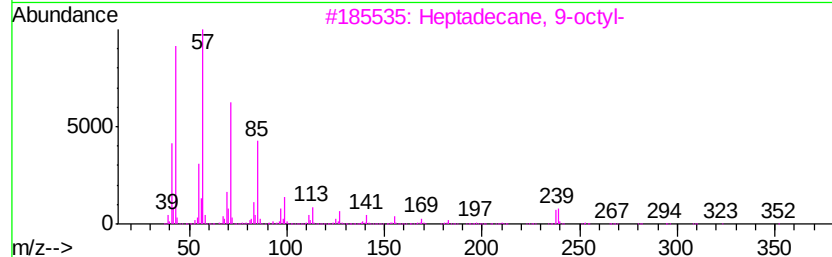
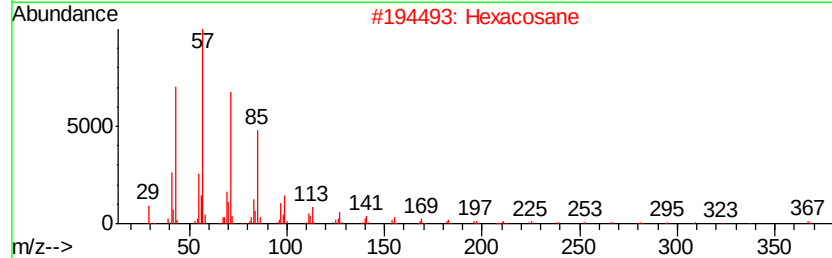
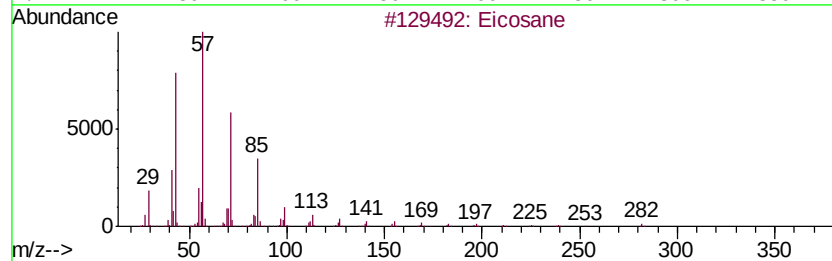
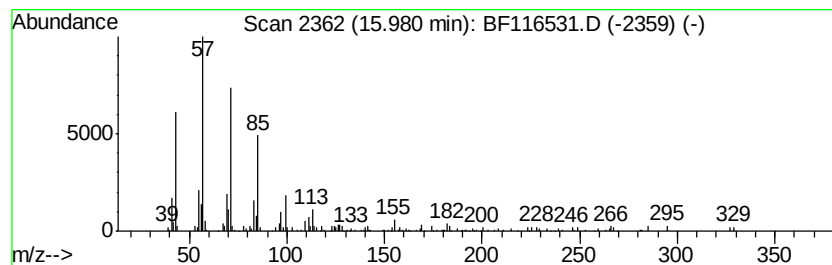
Instrument :
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ClientSampleId :
T9-12-13-K1-K4-(0-1.9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.98	4.66 ng	144114	Perylene-d12		15.50
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Docosane, 7-hexyl-	394	C28H58	055373-86-9	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082519\
Data File : BF116531.D
Acq On : 25 Aug 2019 14:53
Operator : HP/JU
Sample : K4493-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

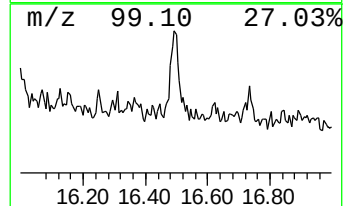
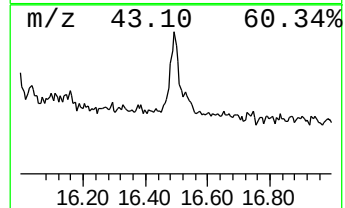
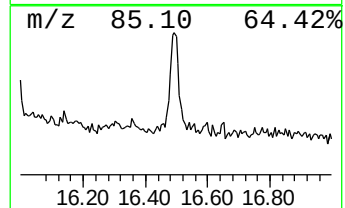
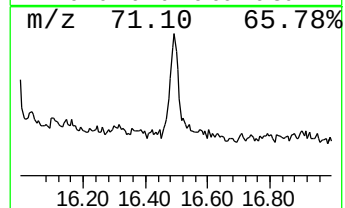
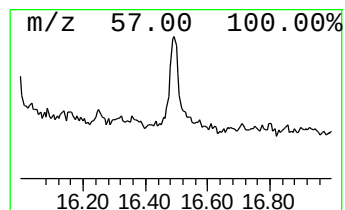
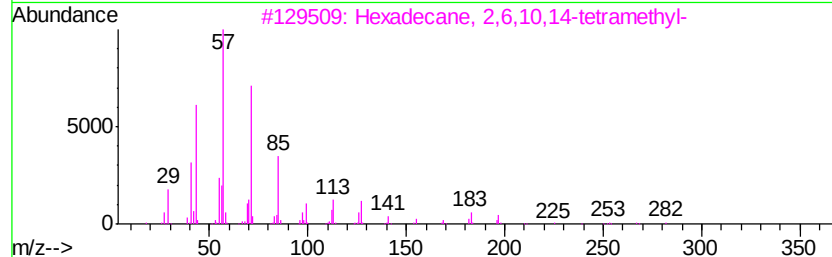
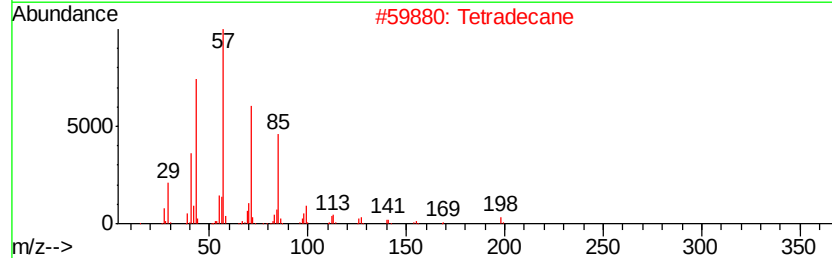
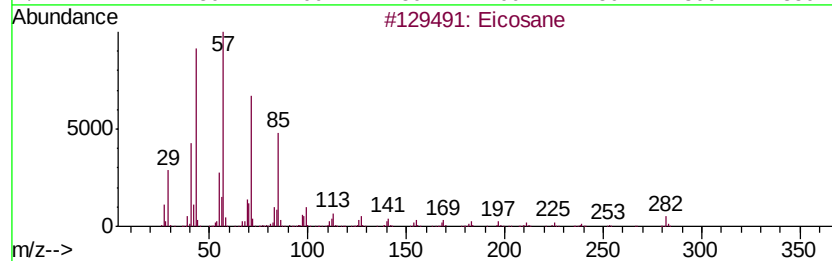
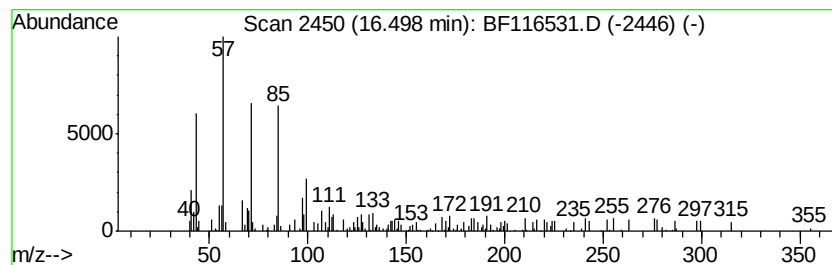
Instrument :
BNA_F
ClientSampleId :
T9-12-13-K1-K4-(0-1.9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.50	2.27 ng	70182	Perylene-d12	15.50
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	83
2	Tetradecane	198 C14H30	000629-59-4	78
3	Hexadecane, 2,6,10,14-tetramethyl-	282 C20H42	000638-36-8	60
4	1-Iodoundecane	282 C11H23I	004282-44-4	58
5	Nonadecane	268 C19H40	000629-92-5	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082519\
Data File : BF116531.D
Acq On : 25 Aug 2019 14:53
Operator : HP/JU
Sample : K4493-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T9-12-13-K1-K4-(0-1.9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.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
Butane, 2-methoxy...	2.25	62.2	ng	2759890	1	6.89	886802	20.0
unknown6.66	6.66	71.7	ng	3179610	1	6.89	886802	20.0
n-Hexadecanoic acid	11.92	3.3	ng	180073	4	11.40	1082930	20.0
1-Heneicosyl formate	13.88	5.3	ng	232211	5	14.03	872923	20.0
Heptadecane	15.16	8.4	ng	259609	6	15.50	618705	20.0
Benzo[e]pyrene	15.37	3.5	ng	107266	6	15.50	618705	20.0
Eicosane	15.98	4.7	ng	144114	6	15.50	618705	20.0
Tetradecane	16.50	2.3	ng	70182	6	15.50	618705	20.0