

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
 Data File : BF114400.D
 Acq On : 18 May 2019 19:16
 Operator : JU/SJ
 Sample : K2896-09
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-20

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-BF051019.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	2.140	3	9	27	rVB	5123550	7250929	100.00%	11.714%
2	5.057	502	505	516	rVB	81309	114804	1.58%	0.185%
3	5.469	571	575	598	rVB	3617133	3680888	50.76%	5.947%
4	6.475	743	746	765	rBV	2492134	2755509	38.00%	4.452%
5	6.610	765	769	773	rBV	5449115	5466907	75.40%	8.832%
6	6.833	804	807	815	rBV	1793772	1549192	21.37%	2.503%
7	6.992	830	834	844	rBV	5180481	4829491	66.61%	7.802%
8	7.369	894	898	899	rBV	132522	120496	1.66%	0.195%
9	7.398	899	903	913	rVV	4064972	4515677	62.28%	7.295%
10	7.475	913	916	919	rVV3	82136	76814	1.06%	0.124%
11	7.522	919	924	927	rVB	73820	79692	1.10%	0.129%
12	7.604	933	938	942	rVB2	139059	139678	1.93%	0.226%
13	7.763	961	965	969	rBV4	78672	110405	1.52%	0.178%
14	7.857	975	981	984	rBV2	312296	339288	4.68%	0.548%
15	8.116	1019	1025	1030	rBV	2173560	2209216	30.47%	3.569%
16	8.163	1030	1033	1036	rVB2	118880	142087	1.96%	0.230%
17	8.233	1042	1045	1049	rBV2	112017	125942	1.74%	0.203%
18	8.357	1062	1066	1068	rBV2	87144	79445	1.10%	0.128%
19	8.774	1133	1137	1140	rBV	149991	134963	1.86%	0.218%
20	8.933	1158	1164	1166	rBV2	61423	91460	1.26%	0.148%
21	9.033	1173	1181	1183	rBV4	53215	107150	1.48%	0.173%
22	9.186	1202	1207	1211	rBV	6470388	6945926	95.79%	11.221%
23	9.527	1259	1265	1271	rBV3	74423	149562	2.06%	0.242%
24	9.580	1271	1274	1278	rVB	254422	236493	3.26%	0.382%
25	9.869	1318	1323	1327	rBV	2206549	2095122	28.89%	3.385%
26	10.274	1389	1392	1397	rVB3	49522	74969	1.03%	0.121%
27	10.657	1453	1457	1464	rBV	3911427	4158119	57.35%	6.718%
28	10.851	1485	1490	1495	rBV4	41094	86778	1.20%	0.140%
29	11.016	1515	1518	1522	rBV2	96124	89937	1.24%	0.145%
30	11.351	1571	1575	1579	rBV	2414631	2167084	29.89%	3.501%
31	11.457	1590	1593	1600	rBV	74321	95357	1.32%	0.154%
32	11.798	1648	1651	1658	rBV3	98410	131791	1.82%	0.213%
33	11.874	1661	1664	1678	rVV2	947552	1042581	14.38%	1.684%
34	12.580	1779	1784	1789	rBV4	64863	115935	1.60%	0.187%

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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-BF051019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.657	1794	1797	1806	rBV	285859	351068	4.84%	0.567%
36	12.933	1839	1844	1848	rBV	5738790	6273593	86.52%	10.135%
37	13.827	1992	1996	2006	rBV	264157	415845	5.74%	0.672%
38	13.992	2020	2024	2031	rVB	1445676	1401848	19.33%	2.265%
39	14.445	2098	2101	2104	rBV	110043	101448	1.40%	0.164%
40	14.745	2149	2152	2157	rVB	144520	139234	1.92%	0.225%
41	15.080	2205	2209	2216	rVB	170005	201519	2.78%	0.326%
42	15.456	2268	2273	2283	rVB	1169820	1560491	21.52%	2.521%
43	15.880	2341	2345	2351	rVB	99181	144148	1.99%	0.233%

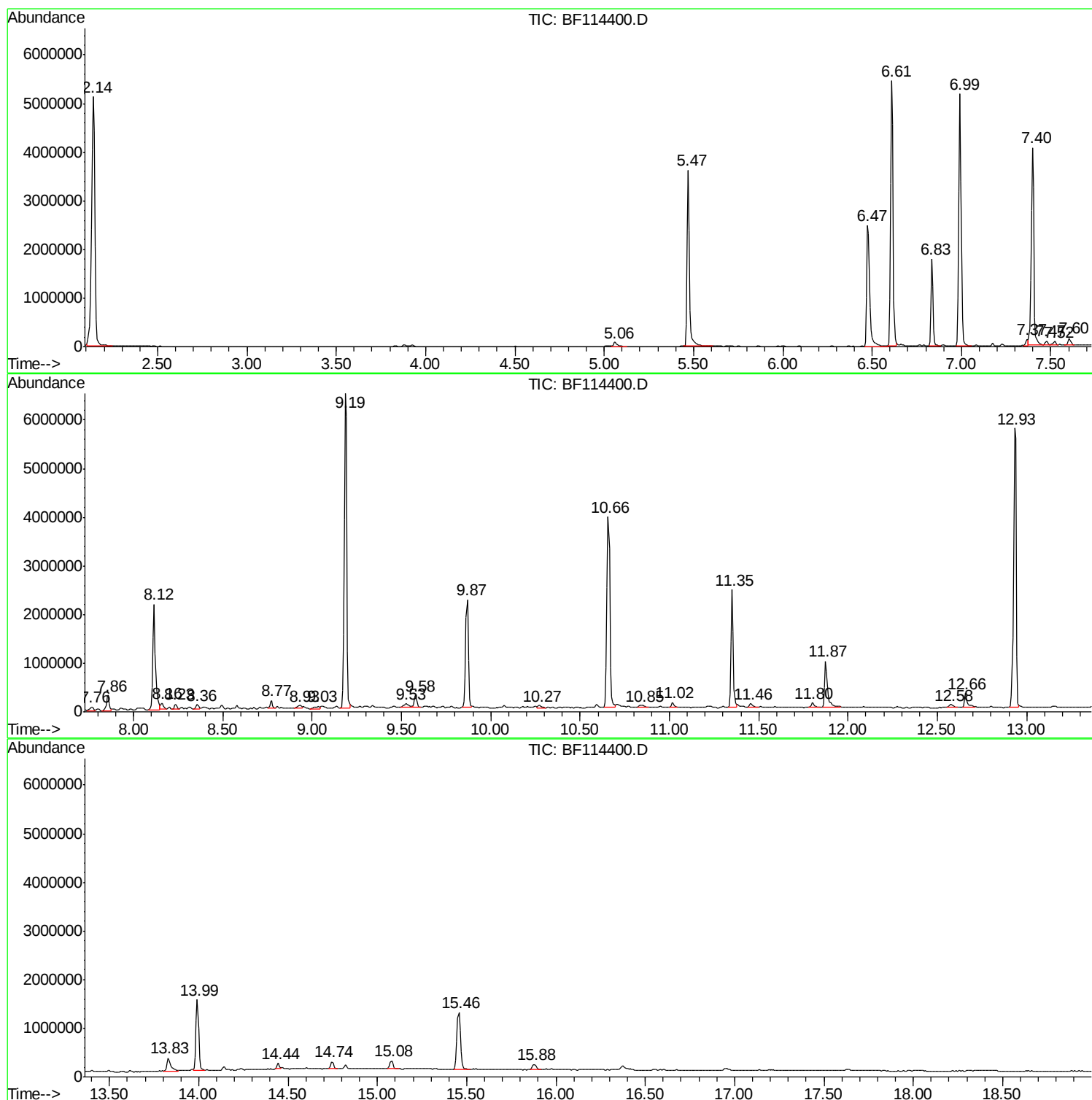
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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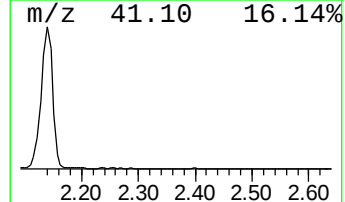
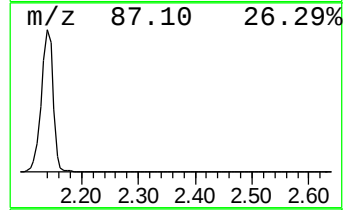
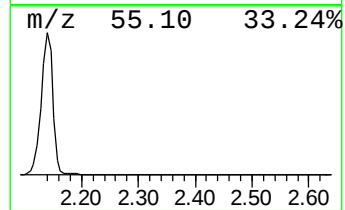
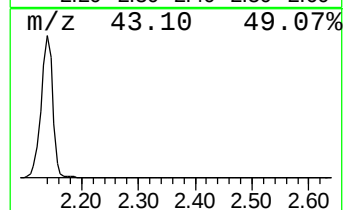
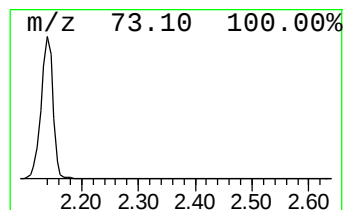
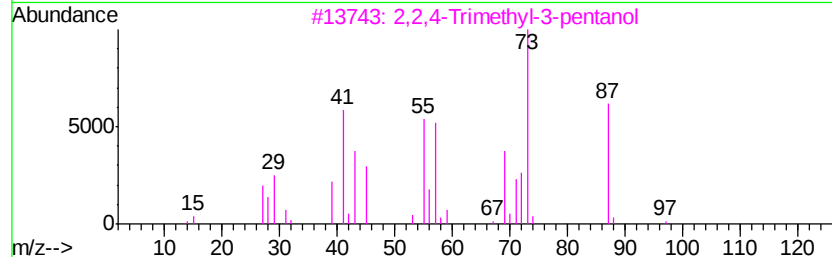
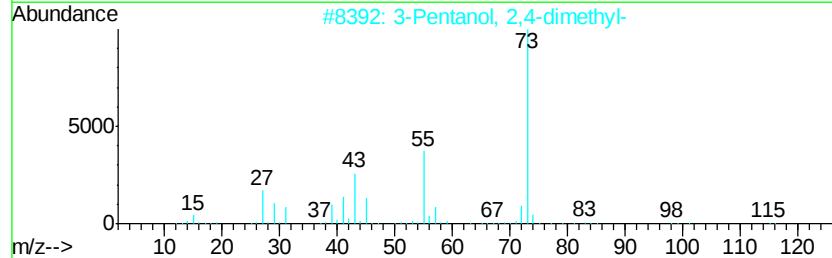
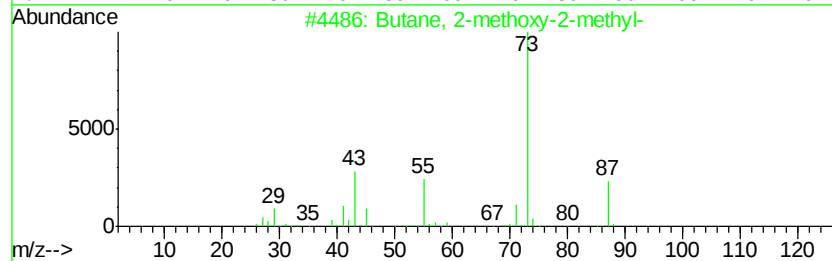
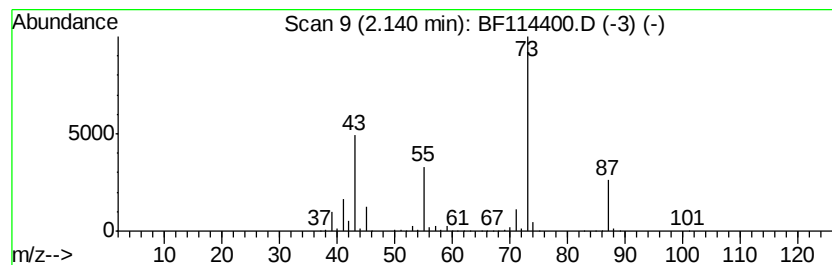
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	93.61 ng	7250930	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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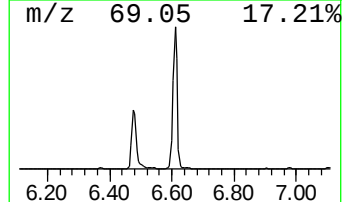
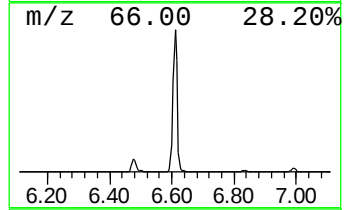
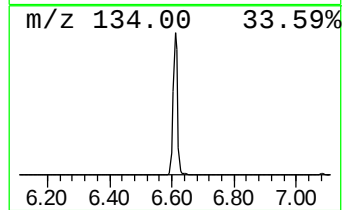
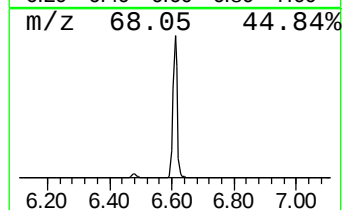
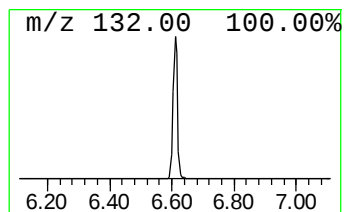
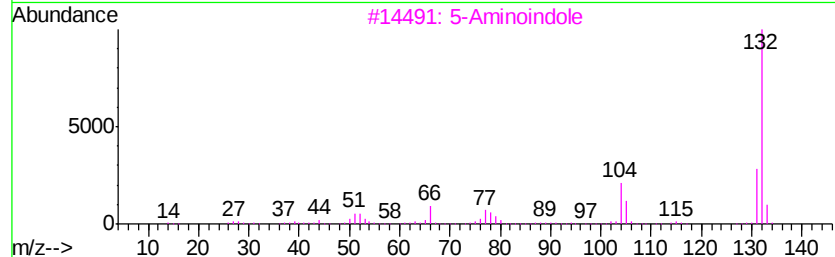
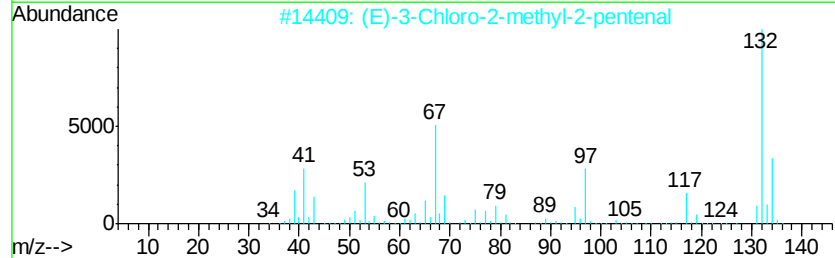
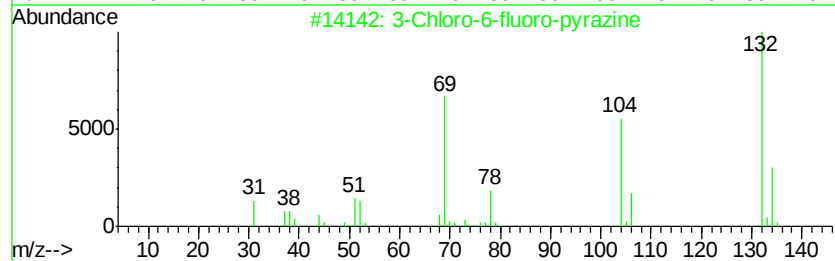
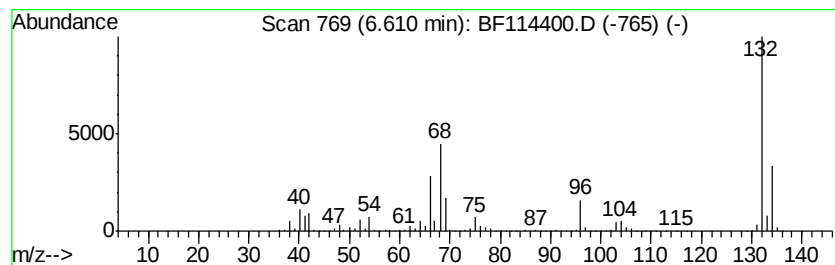
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.61 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	70.58 ng	5466910	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9



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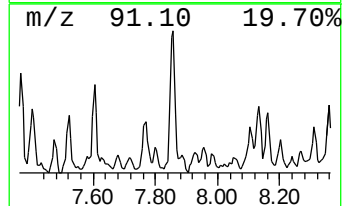
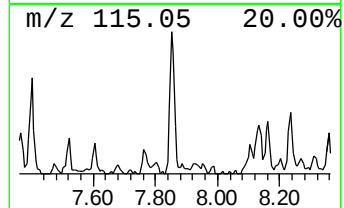
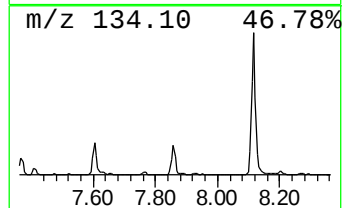
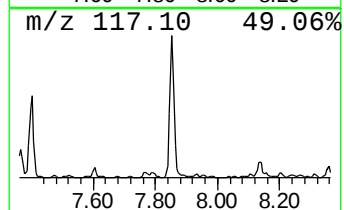
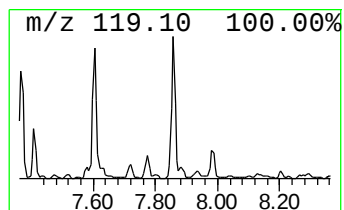
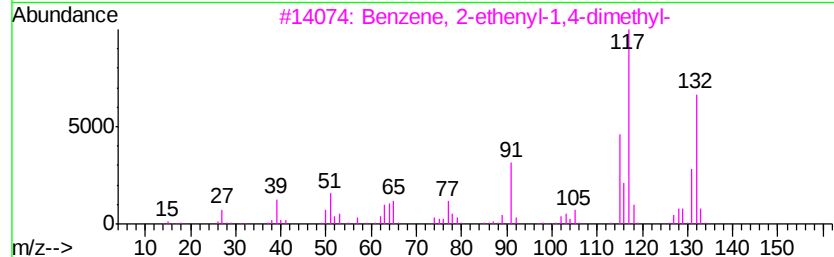
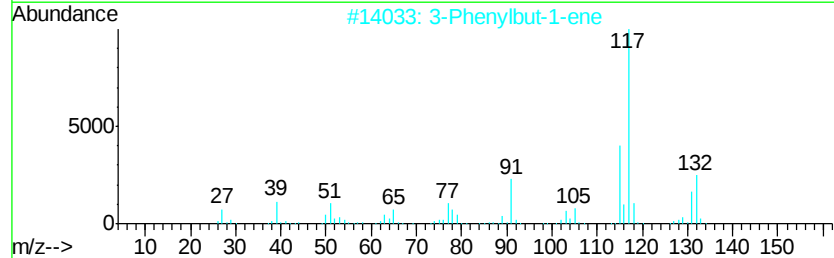
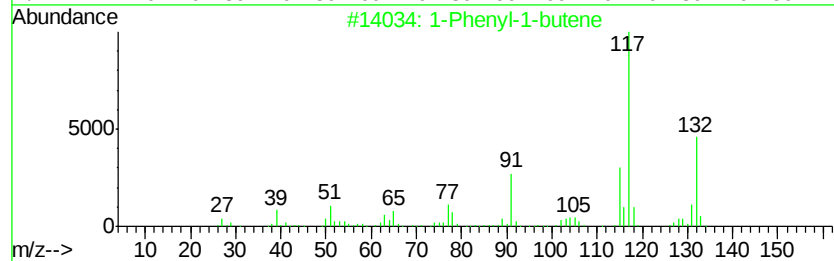
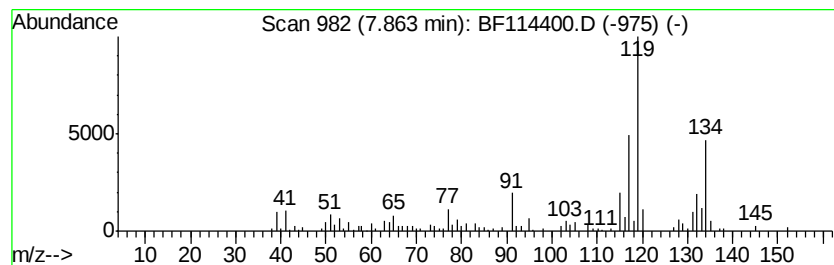
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Phenyl-1-butene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.86	3.07 ng	339288	Naphthalene-d8	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Phenyl-1-butene	132	C10H12	000824-90-8	90
2		3-Phenylbut-1-ene	132	C10H12	000934-10-1	86
3		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	80
4		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	64
5		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	50



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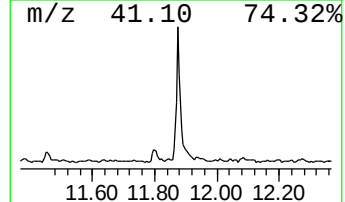
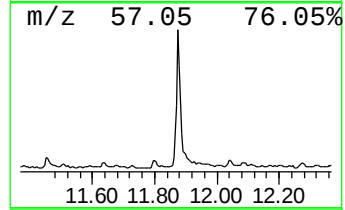
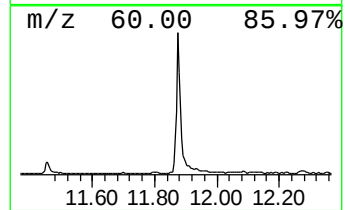
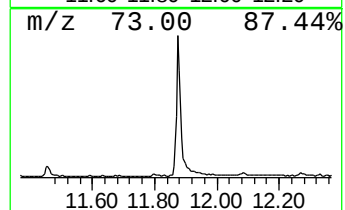
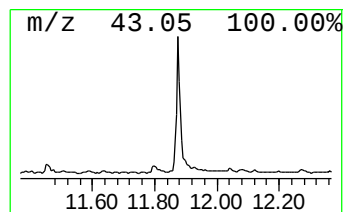
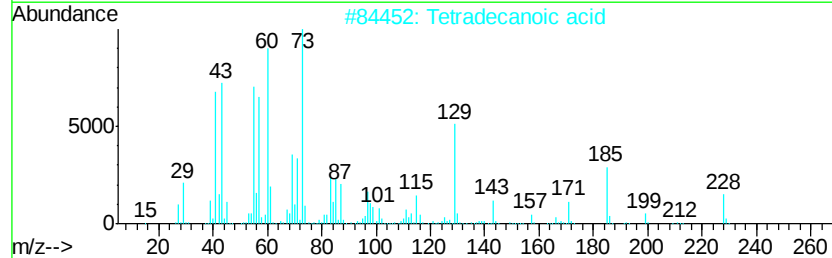
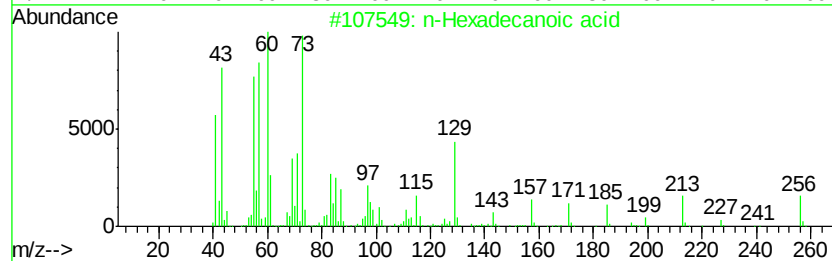
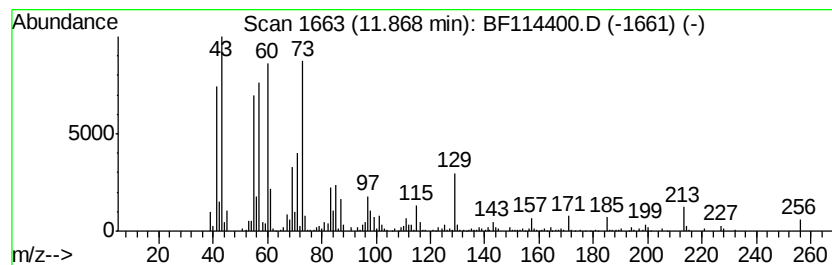
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	9.62 ng	1042580	Phenanthrene-d10	11.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tridecanoic acid	214	C13H26O2	000638-53-9	87
5		Undecanoic acid	186	C11H22O2	000112-37-8	81



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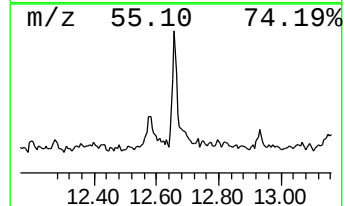
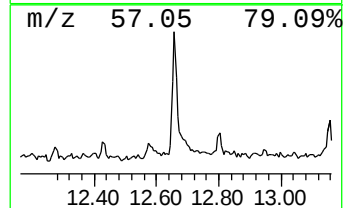
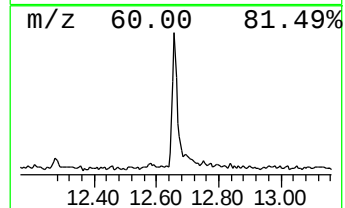
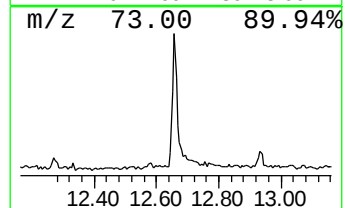
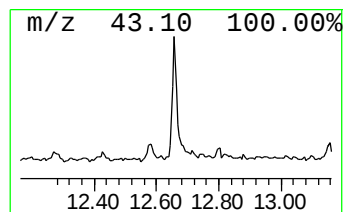
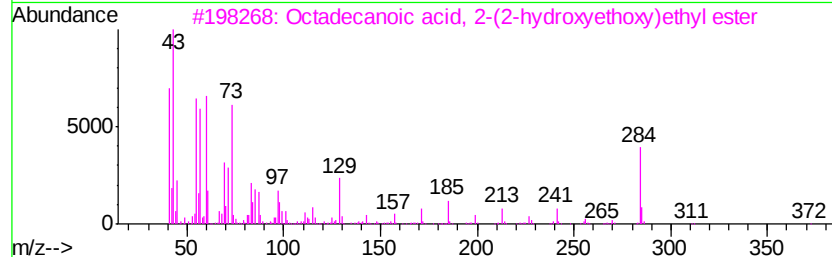
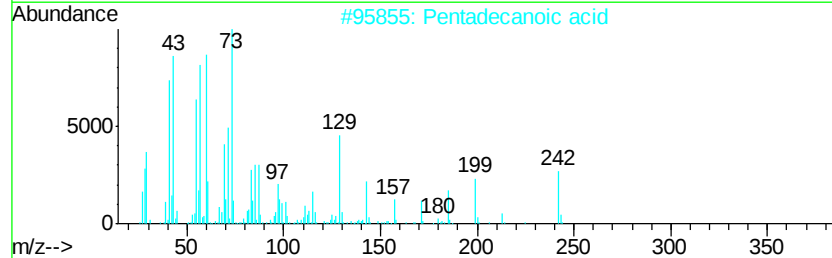
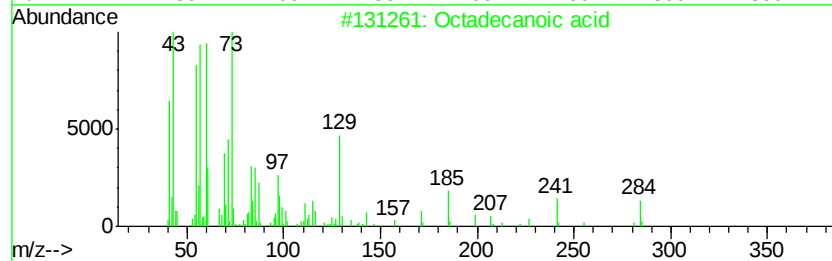
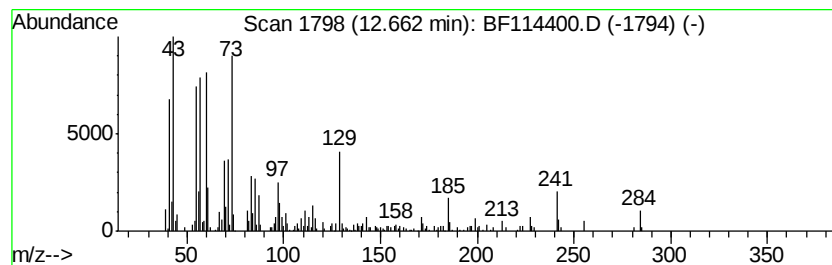
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.66	3.24 ng	351068	Phenanthrene-d10	11.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
Data File : BF114400.D
Acq On : 18 May 2019 19:16
Operator : JU/SJ
Sample : K2896-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

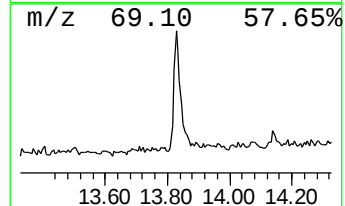
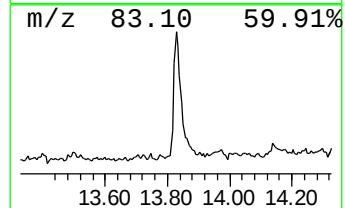
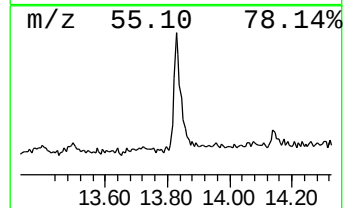
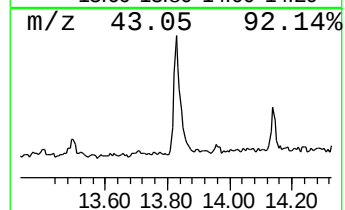
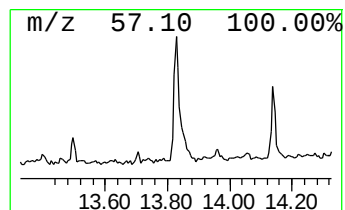
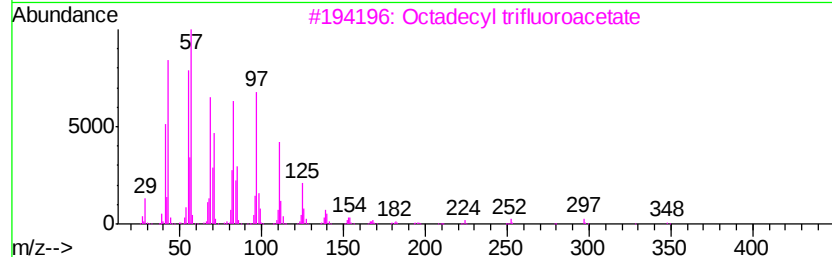
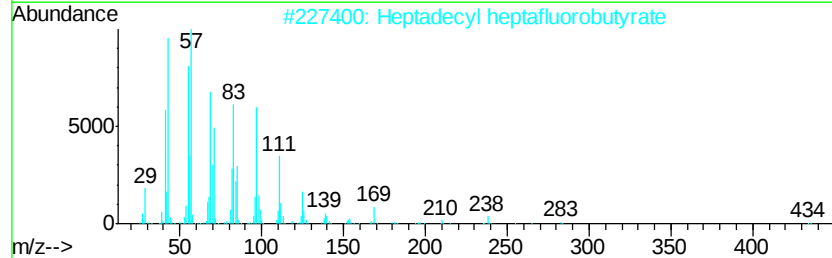
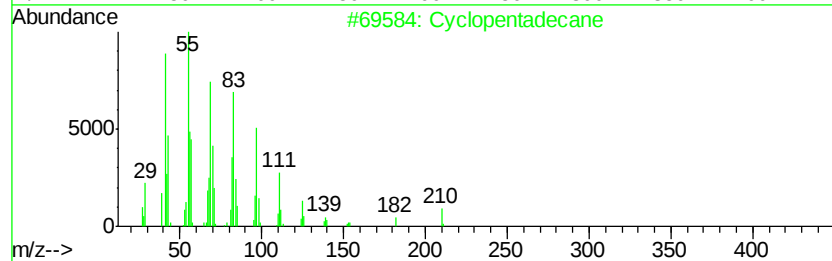
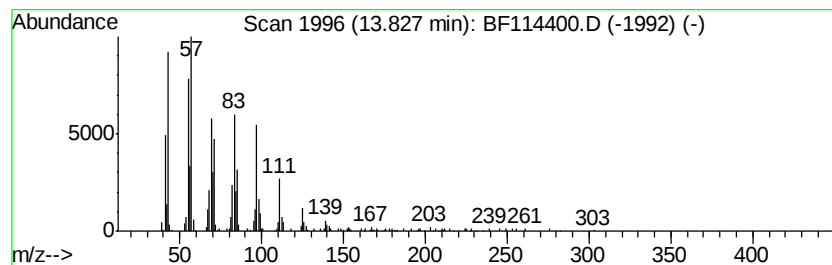
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclopentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.83	5.93 ng	415845	Chrysene-d12		13.99	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentadecane	210	C15H30	000295-48-7	94
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
5		Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
Data File : BF114400.D
Acq On : 18 May 2019 19:16
Operator : JU/SJ
Sample : K2896-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-20

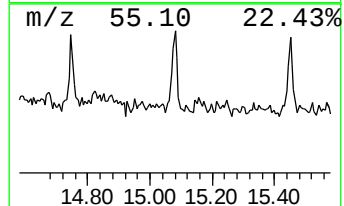
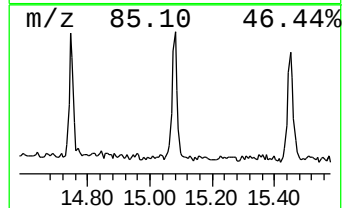
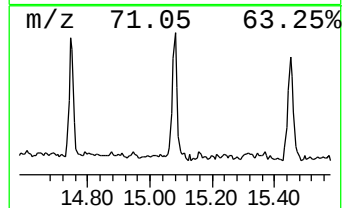
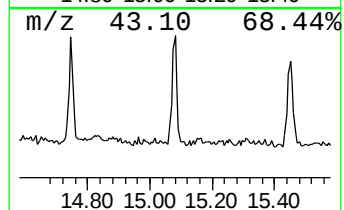
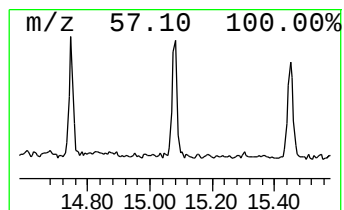
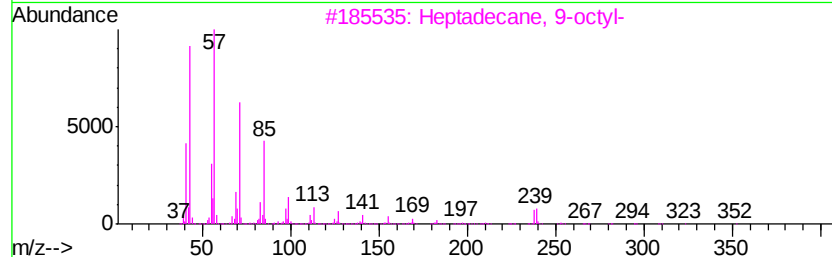
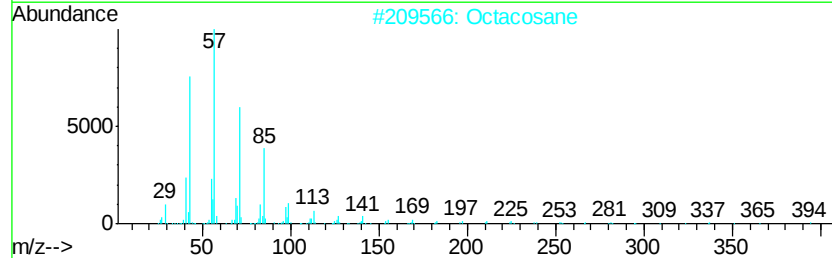
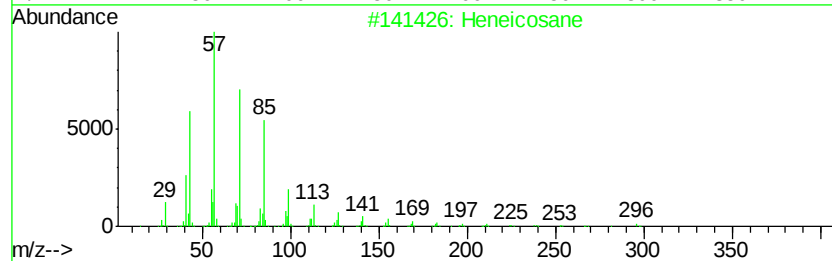
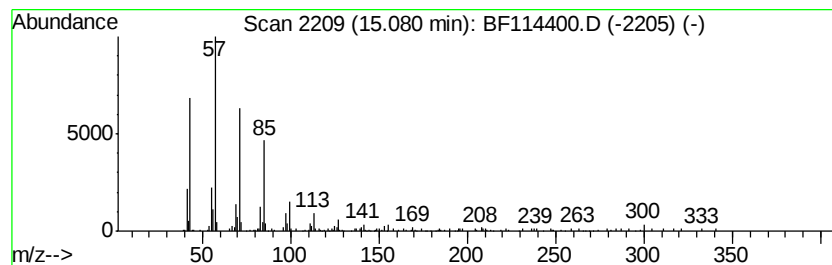
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	2.58 ng	201519	Perylene-d12	15.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	90
2		Octacosane	394	C28H58	000630-02-4	90
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4		Tetracosane	338	C24H50	000646-31-1	87
5		Heptacosane	380	C27H56	000593-49-7	87



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Acq On : 18 May 2019 19:16
Operator : JU/SJ
Sample : K2896-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-20

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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...	2.14	93.6	ng	7250930	1	6.83	1549190	20.0
unknown6.61	6.61	70.6	ng	5466910	1	6.83	1549190	20.0
1-Phenyl-1-butene	7.86	3.1	ng	339288	2	8.12	2209220	20.0
n-Hexadecanoic acid	11.87	9.6	ng	1042580	4	11.35	2167080	20.0
Octadecanoic acid	12.66	3.2	ng	351068	4	11.35	2167080	20.0
Cyclopentadecane	13.83	5.9	ng	415845	5	13.99	1401850	20.0
Heneicosane	15.08	2.6	ng	201519	6	15.46	1560490	20.0