

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF021919\
 Data File : BF112629.D
 Acq On : 19 Feb 2019 19:05
 Operator : JU/SJ
 Sample : K1515-15
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TS-15

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-BF012519.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	5.046	500	503	517	rBV	62078	93903	3.60%	0.430%
2	5.457	569	573	599	rBV	1905444	2041905	78.24%	9.351%
3	6.475	742	746	763	rBV	2007040	2295737	87.97%	10.514%
4	6.598	763	767	780	rVB	2682490	2327612	89.19%	10.660%
5	6.822	801	805	814	rVB	483954	452812	17.35%	2.074%
6	6.975	827	831	846	rBV	1885955	1729529	66.27%	7.921%
7	7.387	897	901	922	rBV	1390675	1376511	52.75%	6.304%
8	8.104	1019	1023	1044	rBV	568991	583989	22.38%	2.675%
9	9.175	1201	1205	1215	rBV	2874094	2558427	98.03%	11.717%
10	9.575	1269	1273	1279	rBV	111136	115650	4.43%	0.530%
11	9.857	1317	1321	1332	rVB	776584	702354	26.91%	3.217%
12	10.651	1452	1456	1471	rBV	1827283	1857083	71.16%	8.505%
13	11.345	1571	1574	1584	rBV	655360	743944	28.51%	3.407%
14	11.863	1659	1662	1675	rBV2	139426	170974	6.55%	0.783%
15	12.651	1793	1796	1806	rBV3	22270	32540	1.25%	0.149%
16	12.927	1838	1843	1846	rBV	2975972	2609730	100.00%	11.952%
17	13.139	1873	1879	1883	rBV3	25796	32509	1.25%	0.149%
18	13.486	1933	1938	1940	rBV2	35383	35233	1.35%	0.161%
19	13.810	1989	1993	2007	rBV	183733	272143	10.43%	1.246%
20	13.992	2021	2024	2032	rBV	625876	645124	24.72%	2.954%
21	14.127	2043	2047	2051	rBV	65191	56192	2.15%	0.257%
22	14.433	2095	2099	2101	rBV	81747	80203	3.07%	0.367%
23	14.733	2145	2150	2154	rBV	83114	86892	3.33%	0.398%
24	14.804	2158	2162	2166	rVB	71886	69672	2.67%	0.319%
25	15.063	2201	2206	2210	rBV2	97015	111891	4.29%	0.512%
26	15.433	2262	2269	2271	rBV2	64532	88889	3.41%	0.407%
27	15.468	2271	2275	2283	rVB	372813	515377	19.75%	2.360%
28	15.857	2336	2341	2346	rVB2	57304	82311	3.15%	0.377%
29	16.351	2420	2425	2428	rBV3	22444	35572	1.36%	0.163%
30	16.927	2517	2523	2529	rBV3	12133	30695	1.18%	0.141%

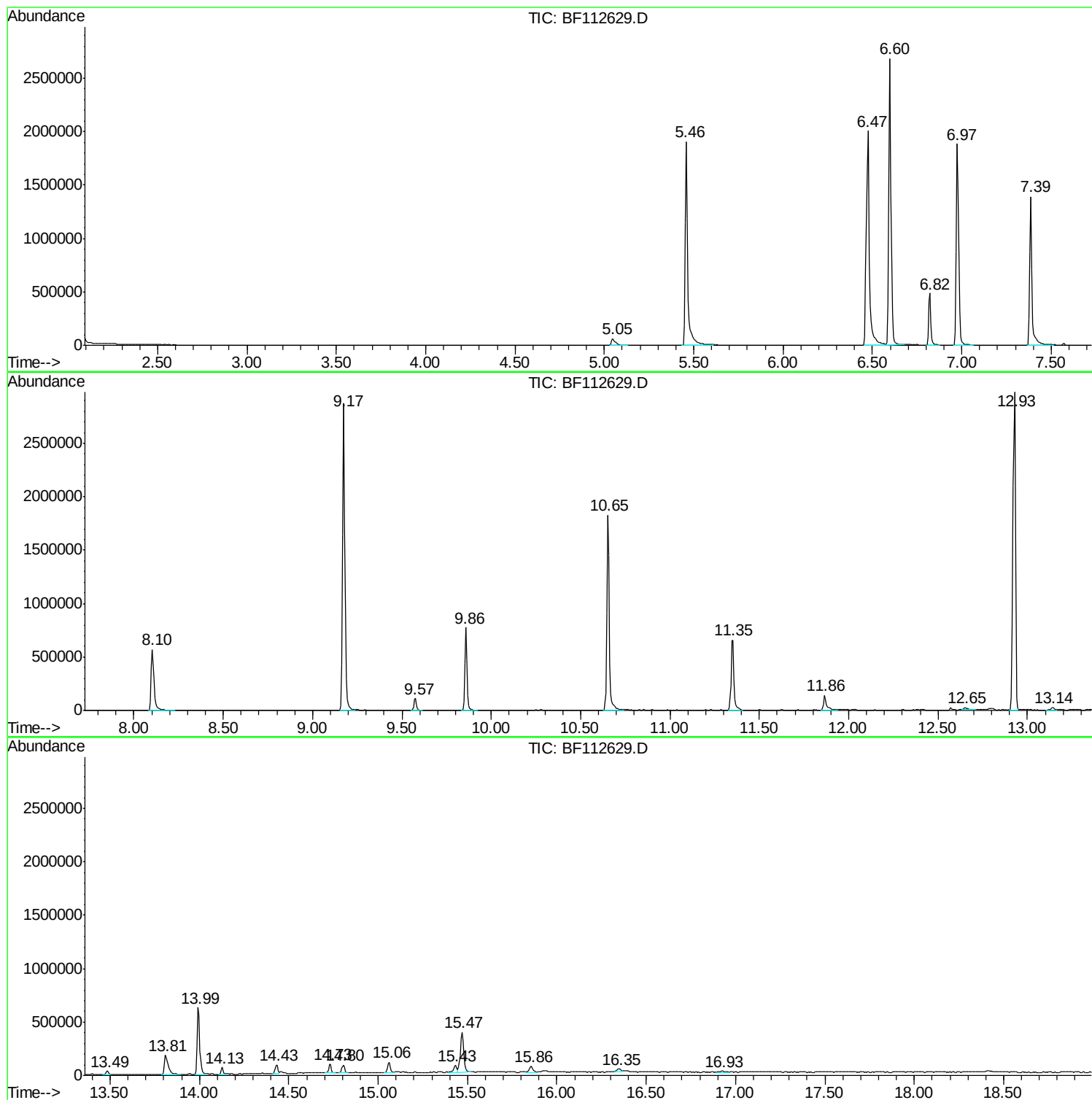
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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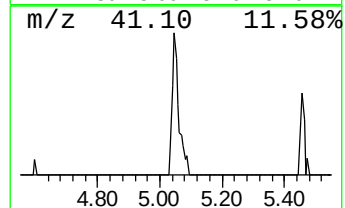
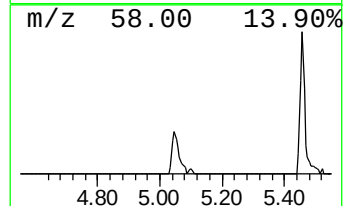
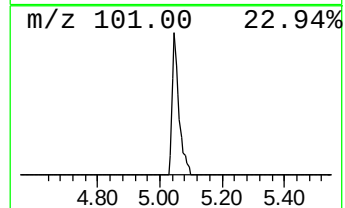
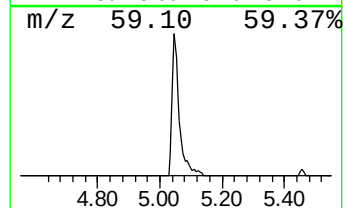
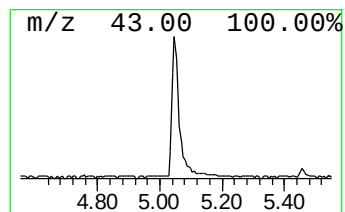
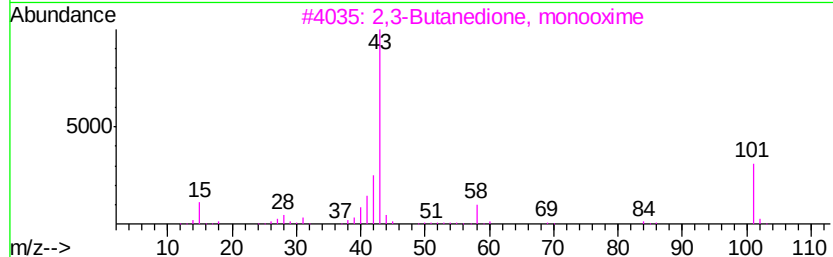
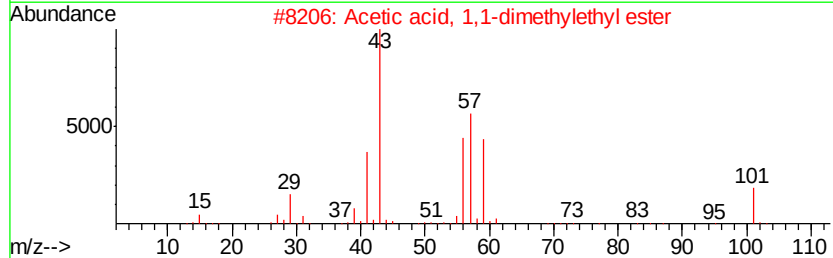
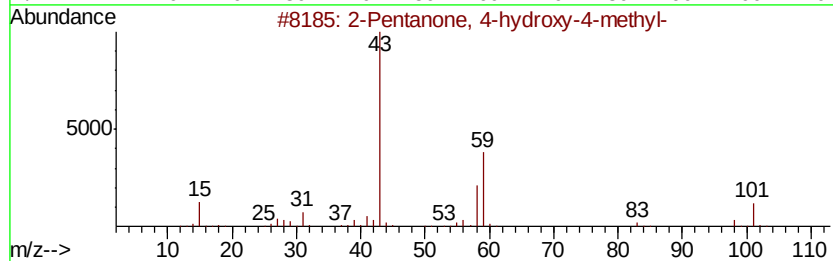
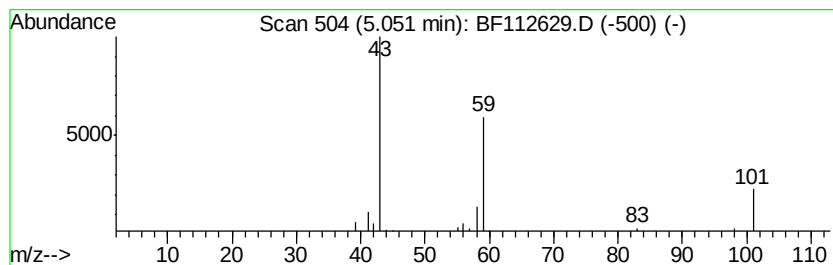
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	4.15 ng	93903	1,4-Dichlorobenzene-d4	6.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
5			Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9



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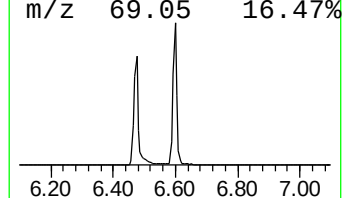
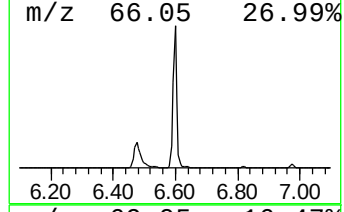
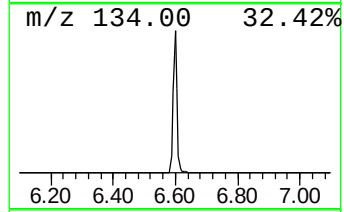
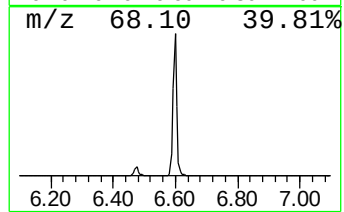
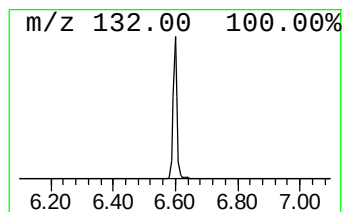
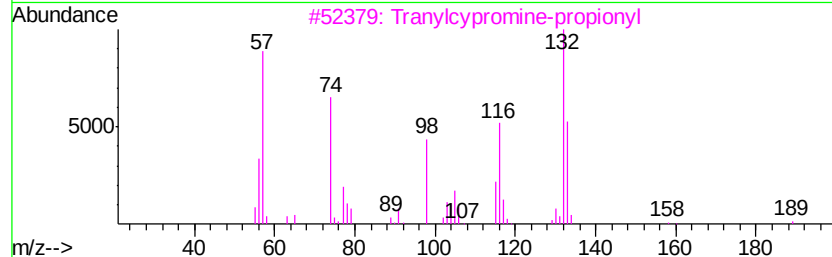
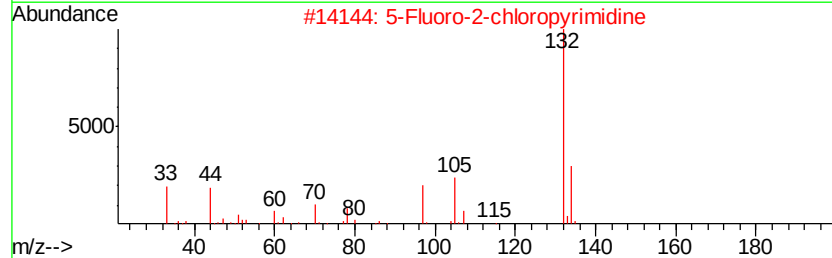
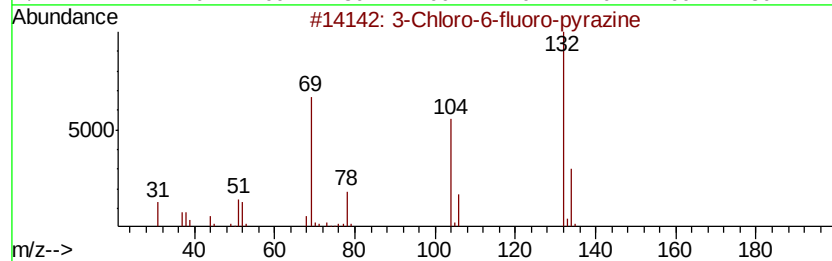
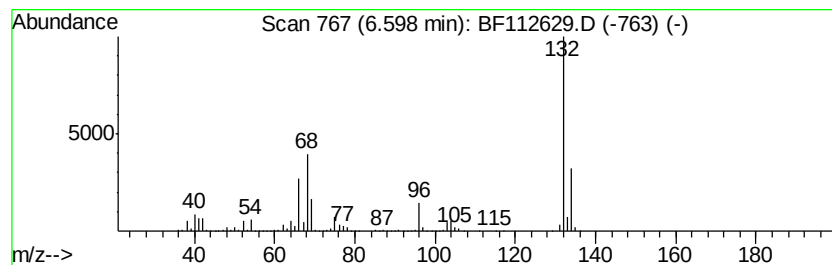
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Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	102.81 ng	2327610	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		Xenon	132	Xe	007440-63-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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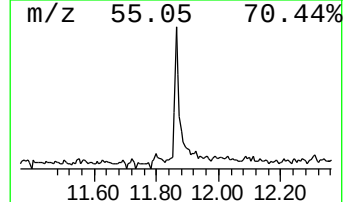
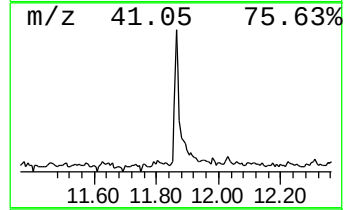
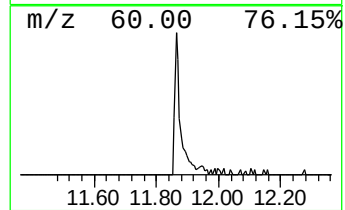
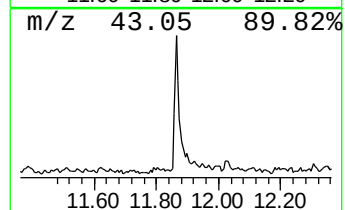
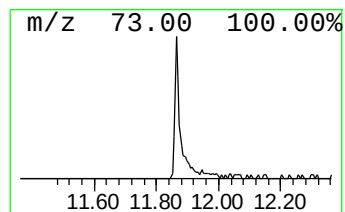
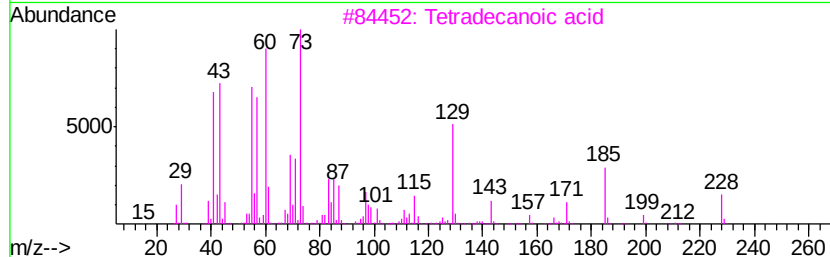
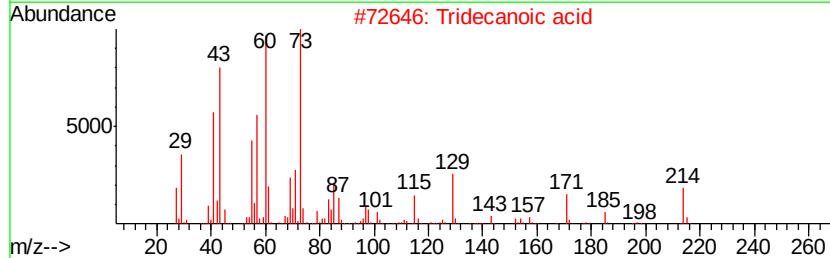
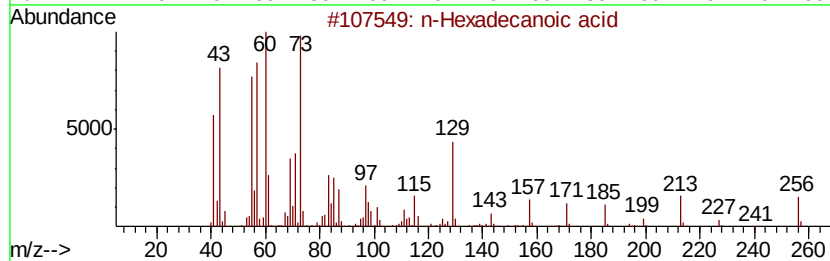
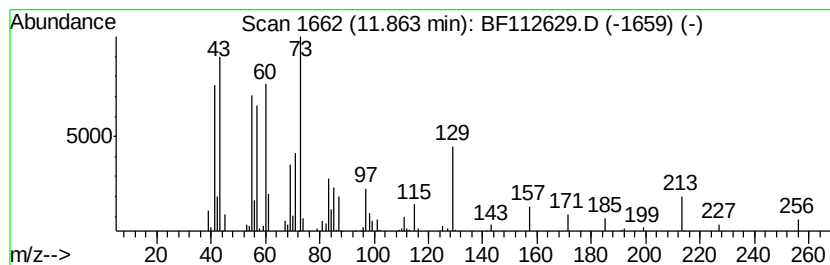
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	4.60 ng	170974	Phenanthrene-d10	11.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	81
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5		Oxalic acid, isobutyl tridecyl e...	328	C19H36O4	1000309-37-8	11



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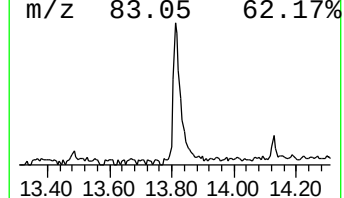
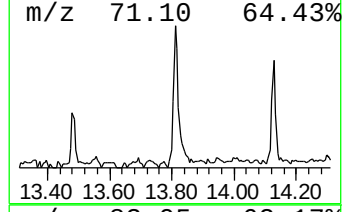
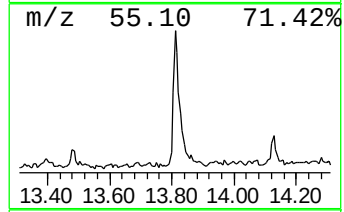
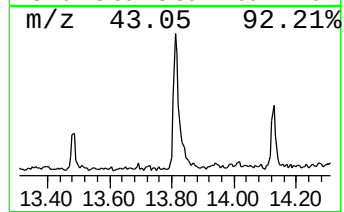
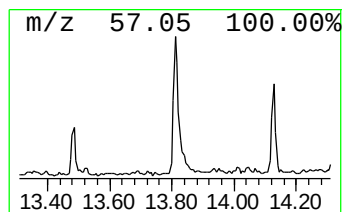
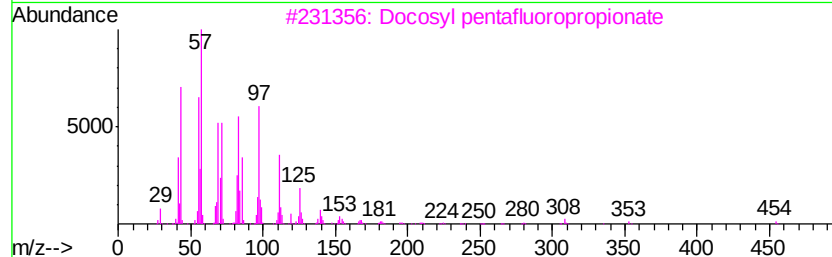
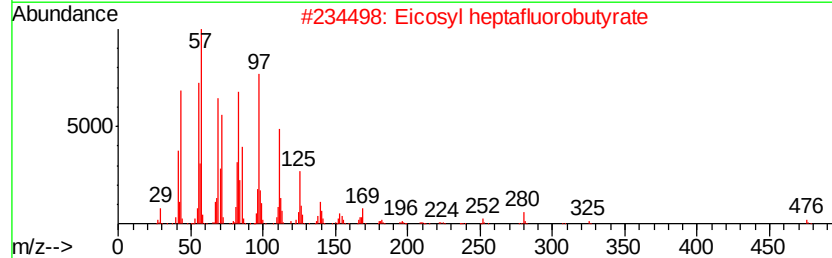
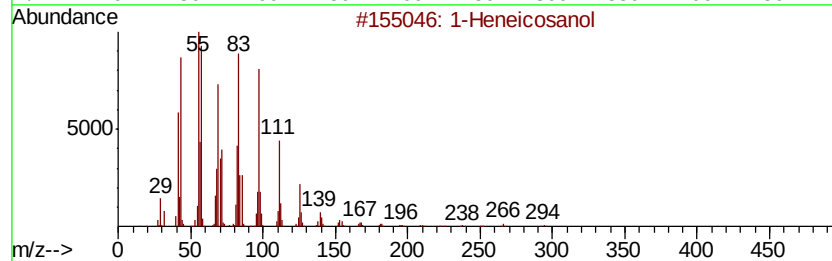
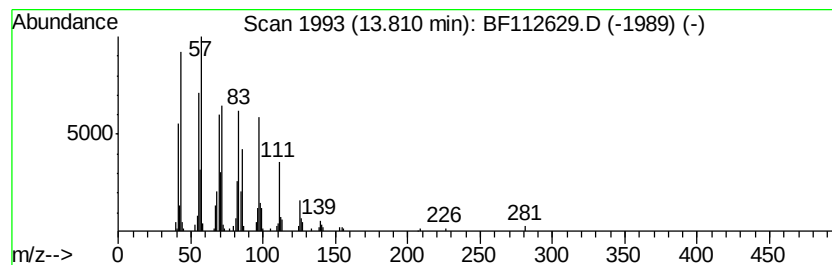
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Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.81	8.44 ng	272143	Chrysene-d12		13.99		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	93
2			Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
3			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
4			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
5			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91



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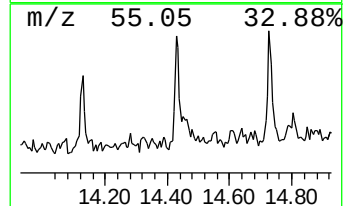
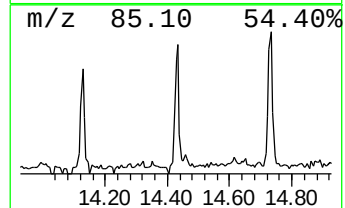
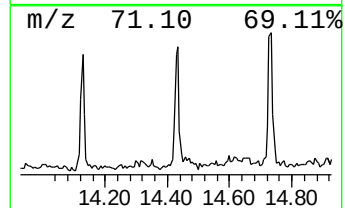
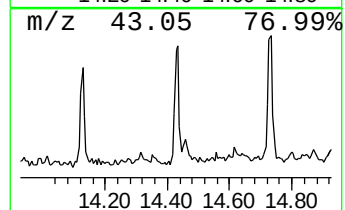
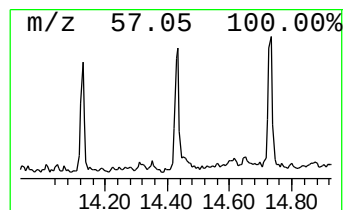
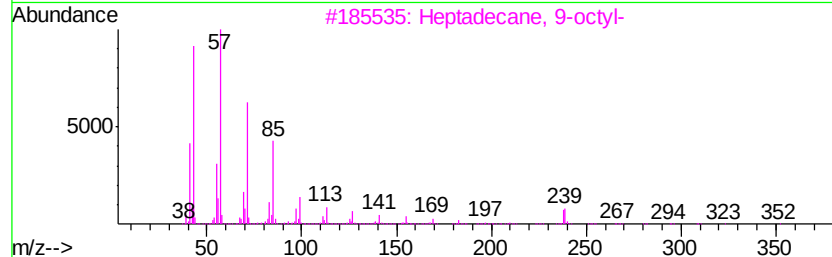
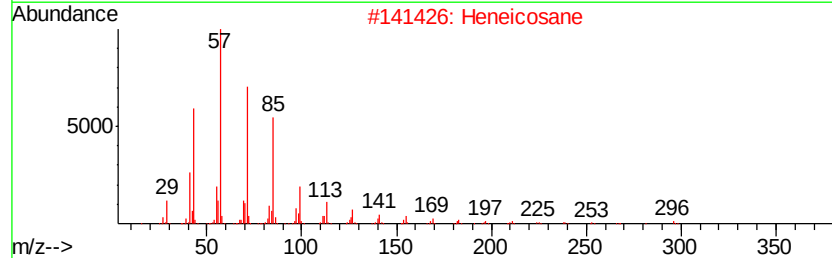
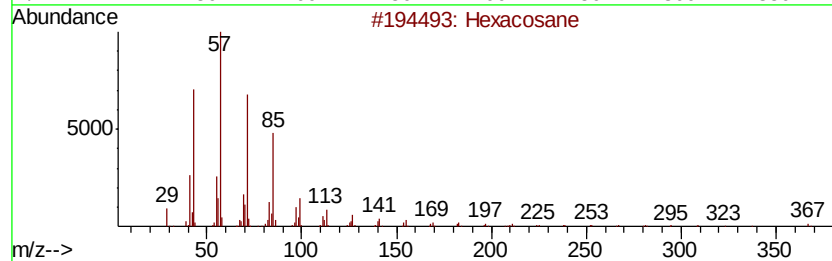
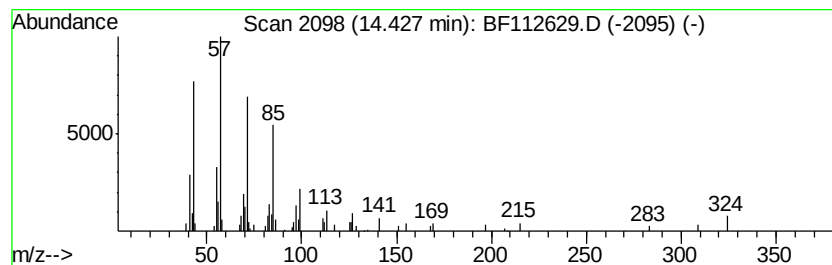
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Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	2.49 ng	80203	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4		Eicosane	282	C20H42	000112-95-8	87
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87



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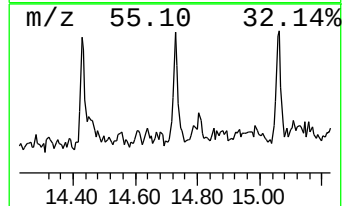
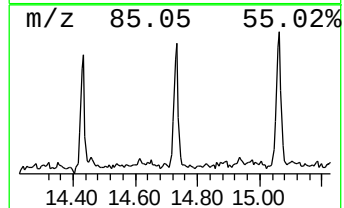
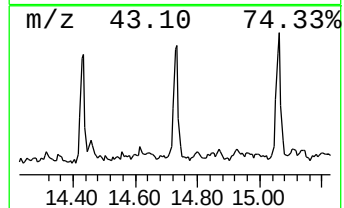
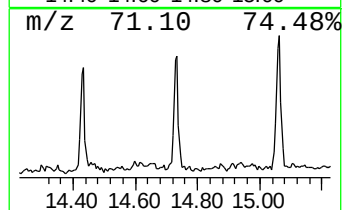
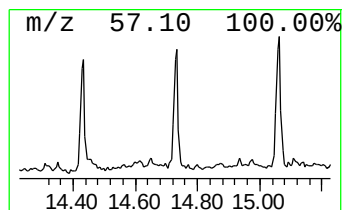
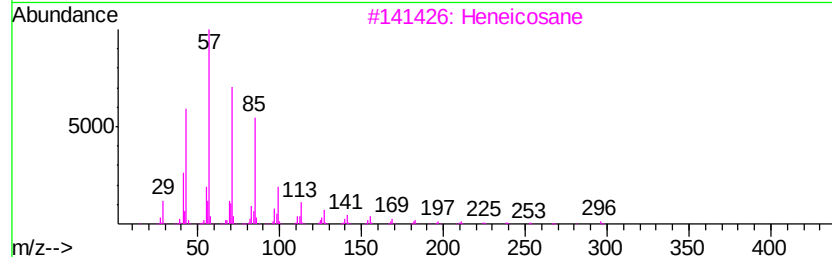
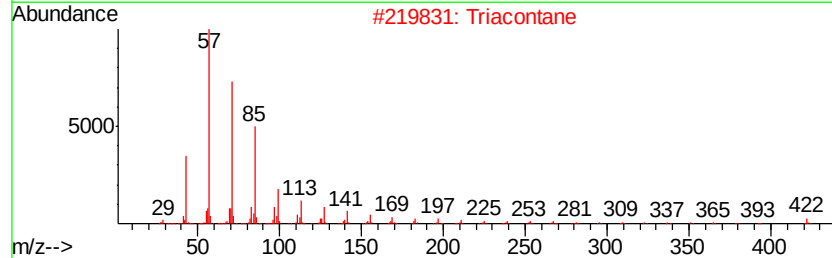
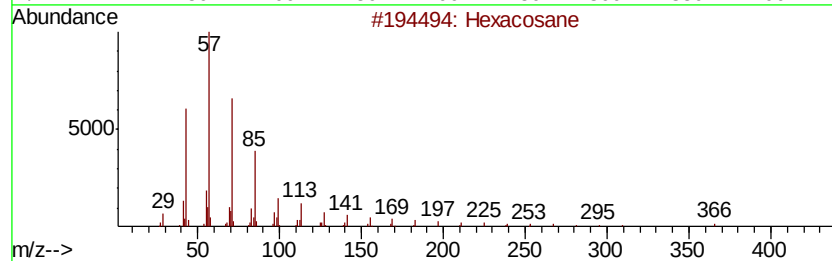
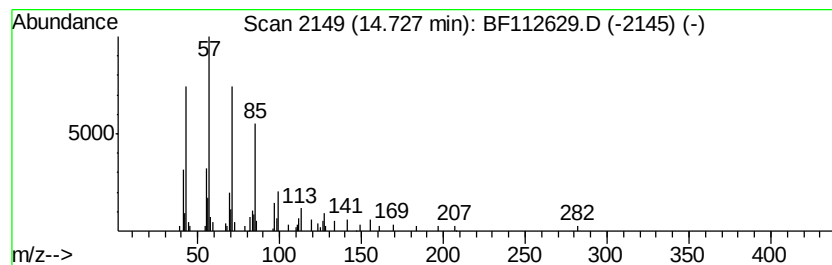
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	3.37 ng	86892	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Triacotane	422	C30H62	000638-68-6	91
3		Heneicosane	296	C21H44	000629-94-7	90
4		Nonacosane	408	C29H60	000630-03-5	90
5		Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021919\
 Data File : BF112629.D
 Acq On : 19 Feb 2019 19:05
 Operator : JU/SJ
 Sample : K1515-15
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TS-15

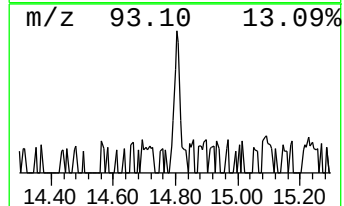
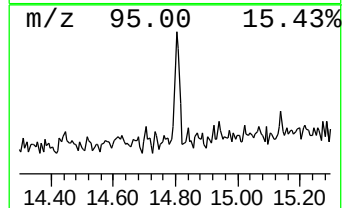
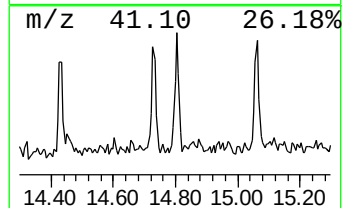
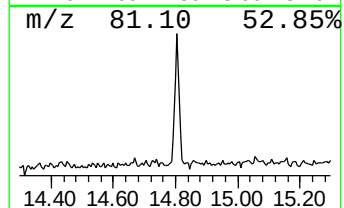
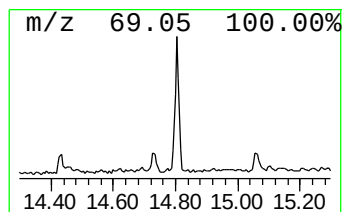
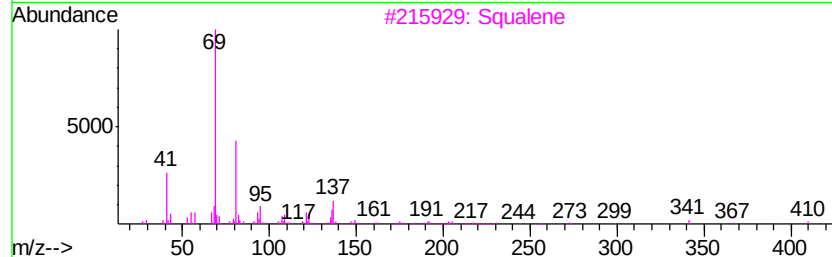
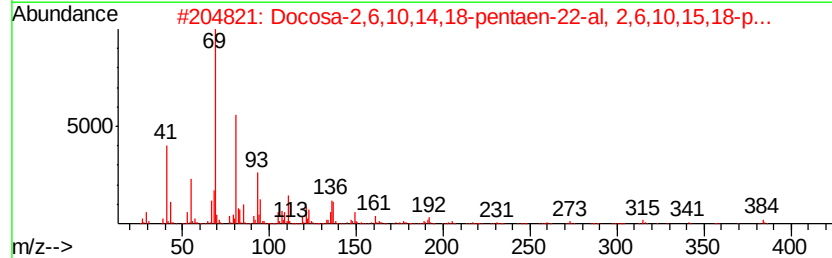
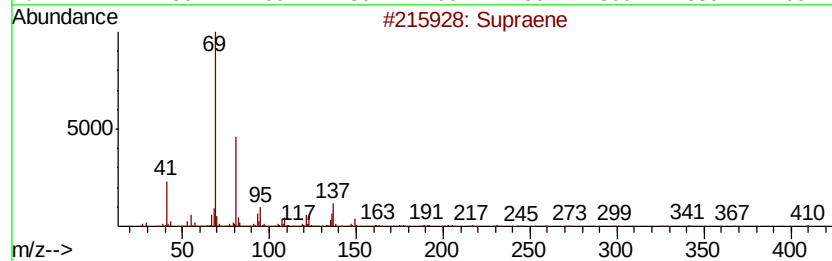
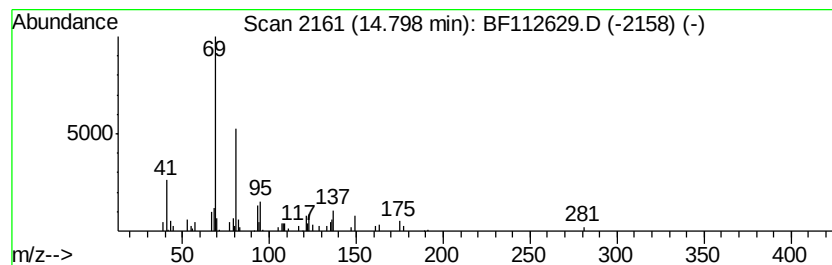
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Supraene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	2.70 ng	69672	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
3		Squalene	410	C30H50	000111-02-4	90
4		trans-Farnesol	222	C15H26O	000106-28-5	72
5		.beta.-d-Mannofuranoside, O-geranyl	316	C16H28O6	1000154-77-2	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021919\
Data File : BF112629.D
Acq On : 19 Feb 2019 19:05
Operator : JU/SJ
Sample : K1515-15
Misc :
ALS Vial : 19 Sample Multiplier: 1

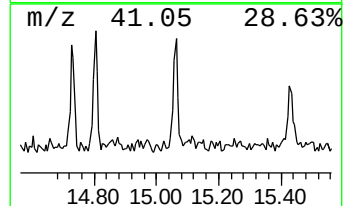
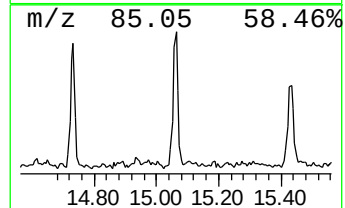
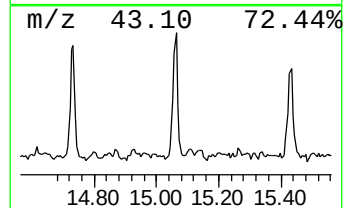
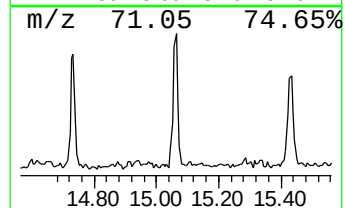
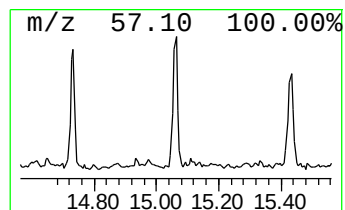
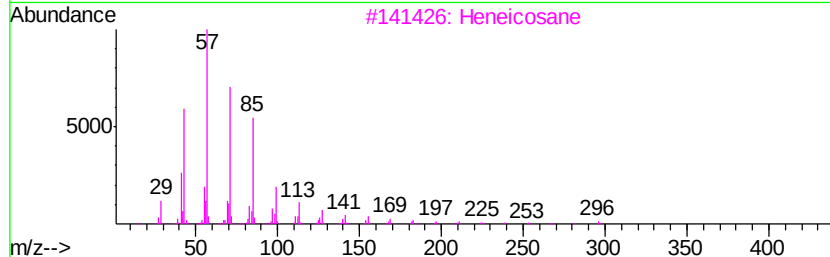
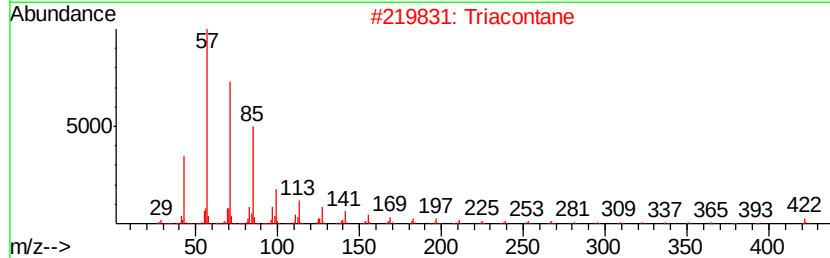
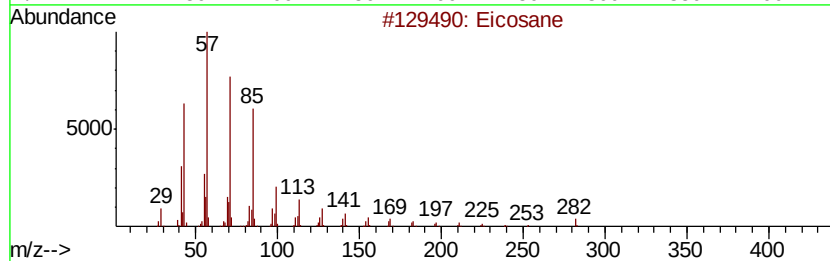
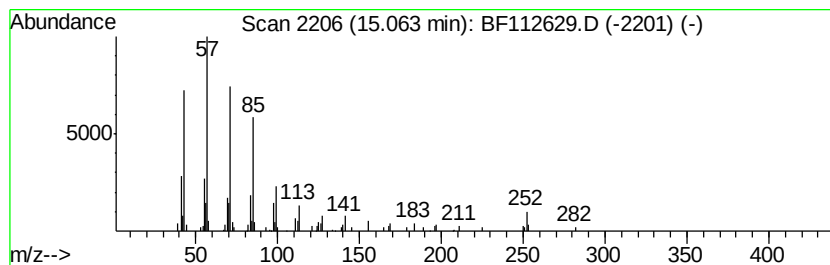
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.06	4.34 ng	111891	Perylene-d12	15.47	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Triacontane	422	C30H62	000638-68-6	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021919\
Data File : BF112629.D
Acq On : 19 Feb 2019 19:05
Operator : JU/SJ
Sample : K1515-15
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TS-15

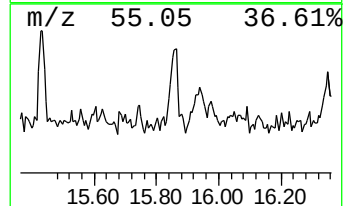
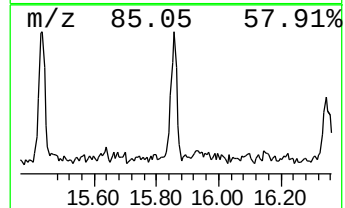
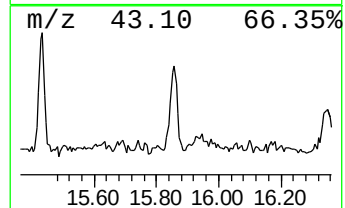
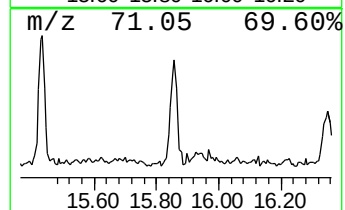
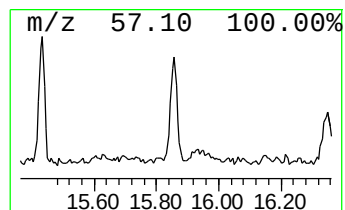
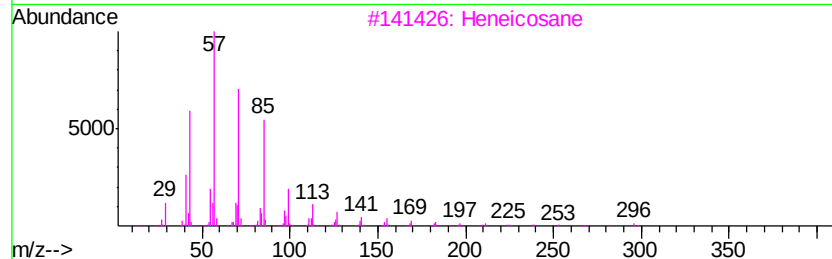
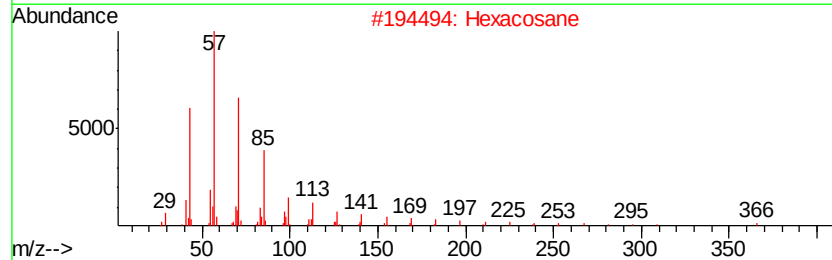
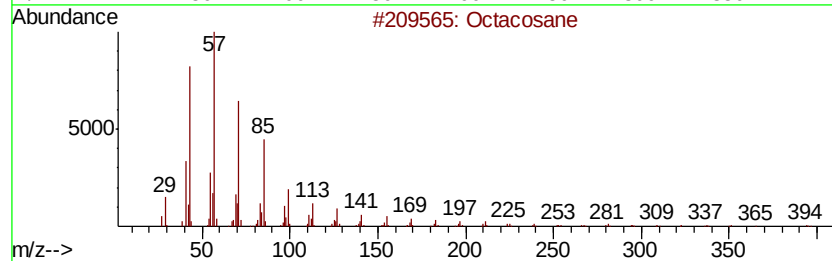
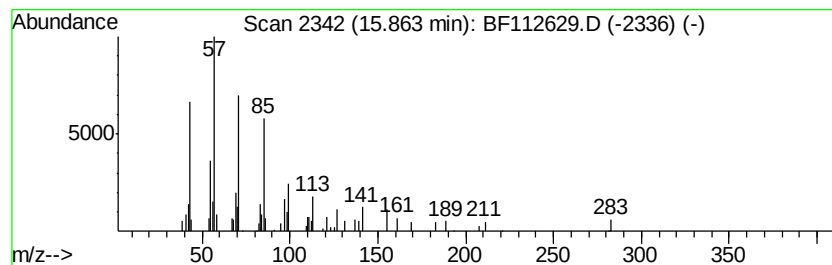
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	3.19 ng	82311	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Pentacosane	352	C25H52	000629-99-2	91
5		Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF021919\
Data File : BF112629.D
Acq On : 19 Feb 2019 19:05
Operator : JU/SJ
Sample : K1515-15
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TS-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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
2-Pentanone, 4-hy...	5.05	4.2	ng	93903	1	6.82	452812	20.0
unknown6.60	6.60	102.8	ng	2327610	1	6.82	452812	20.0
n-Hexadecanoic acid	11.86	4.6	ng	170974	4	11.35	743944	20.0
1-Heneicosanol	13.81	8.4	ng	272143	5	13.99	645124	20.0
Heptadecane, 9-oc...	14.43	2.5	ng	80203	5	13.99	645124	20.0
Hexacosane	14.73	3.4	ng	86892	6	15.47	515377	20.0
Supraene	14.80	2.7	ng	69672	6	15.47	515377	20.0
Eicosane	15.06	4.3	ng	111891	6	15.47	515377	20.0
Octacosane	15.86	3.2	ng	82311	6	15.47	515377	20.0