

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121919\
 Data File : BF118277.D
 Acq On : 19 Dec 2019 14:10
 Operator : JU
 Sample : PB125579BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB125579BL

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-BF120619.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	5.081	504	509	520	rBV	424800	568010	12.20%	1.609%
2	5.487	573	578	581	rBV	3105279	2954905	63.46%	8.368%
3	6.493	744	749	752	rBV	2813180	3106279	66.72%	8.797%
4	6.634	768	773	776	rBV	3684747	3406623	73.17%	9.648%
5	6.857	808	811	821	rBV	842237	678579	14.57%	1.922%
6	7.016	834	838	841	rBV	3198461	2686414	57.70%	7.608%
7	7.422	902	907	921	rBV	1797261	2012111	43.22%	5.698%
8	8.145	1026	1030	1044	rBV	918190	876033	18.82%	2.481%
9	9.228	1208	1214	1217	rBV	4042425	4165884	89.47%	11.798%
10	9.904	1325	1329	1342	rVB	1017224	1054213	22.64%	2.986%
11	10.704	1460	1465	1482	rBV	3048377	2912124	62.55%	8.247%
12	11.398	1580	1583	1591	rBV	1061009	1095896	23.54%	3.104%
13	12.992	1849	1854	1857	rBV	4964633	4655986	100.00%	13.186%
14	14.051	2030	2034	2046	rBV	765460	822522	17.67%	2.329%
15	14.204	2055	2060	2065	rBV	143220	137358	2.95%	0.389%
16	14.510	2105	2112	2117	rBV	344682	335482	7.21%	0.950%
17	14.821	2159	2165	2173	rBV	573639	603661	12.97%	1.710%
18	15.163	2217	2223	2237	rBV	600299	753604	16.19%	2.134%
19	15.398	2258	2263	2276	rVB7	20928	59192	1.27%	0.168%
20	15.551	2282	2289	2299	rBV2	864158	1406620	30.21%	3.984%
21	15.998	2356	2365	2377	rBV	372071	603523	12.96%	1.709%
22	16.510	2444	2452	2461	rBV2	166938	322716	6.93%	0.914%
23	17.115	2549	2555	2564	rVB3	40615	93112	2.00%	0.264%

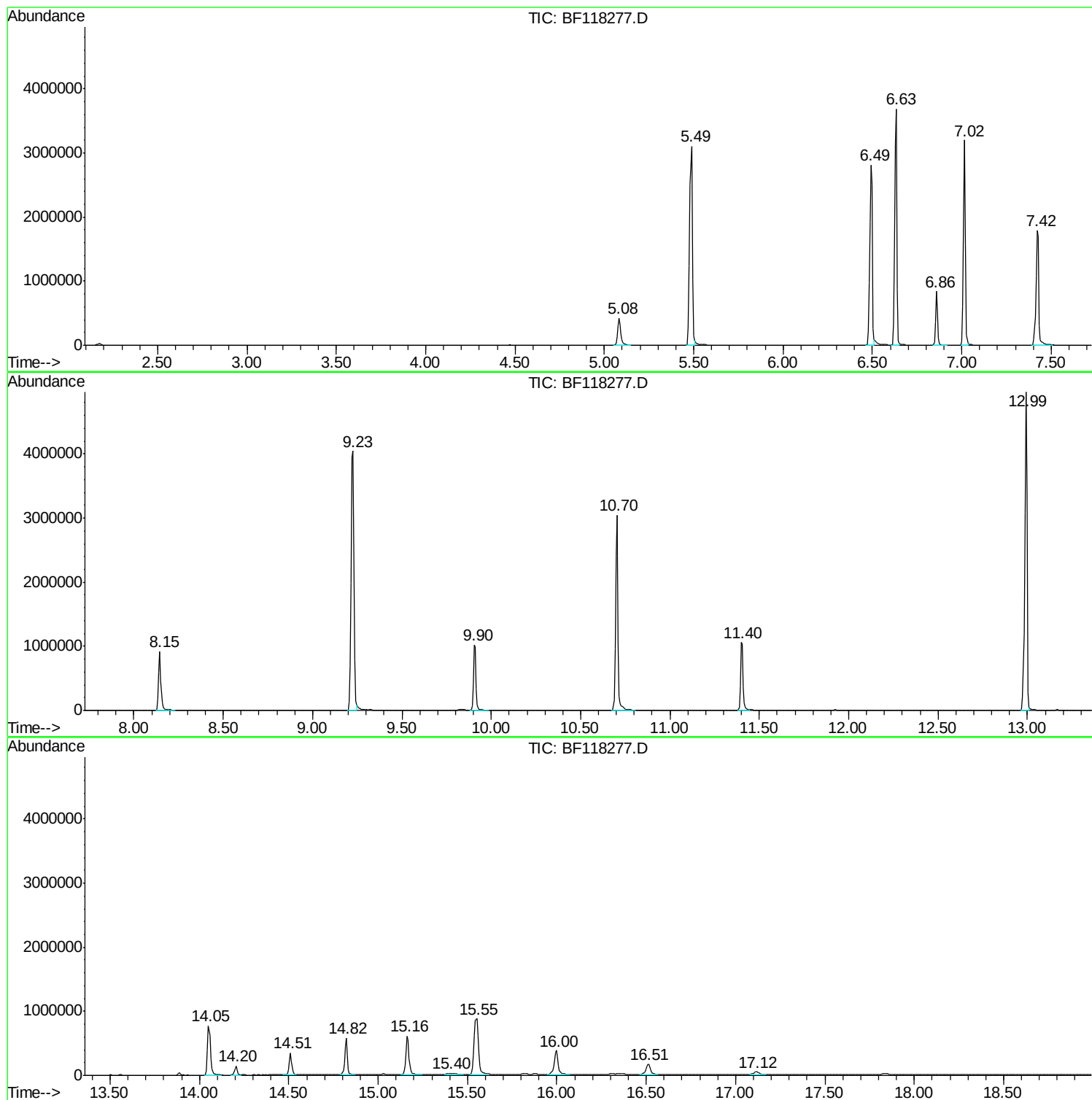
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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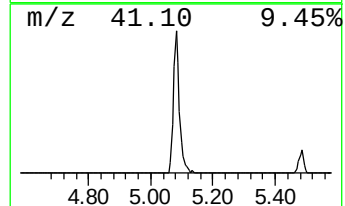
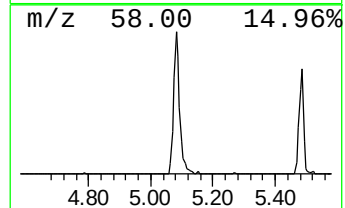
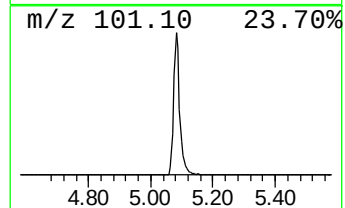
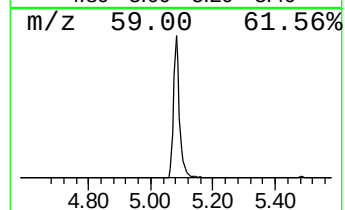
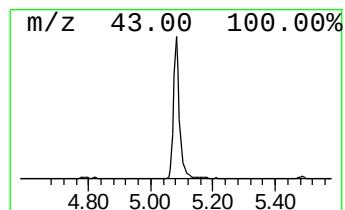
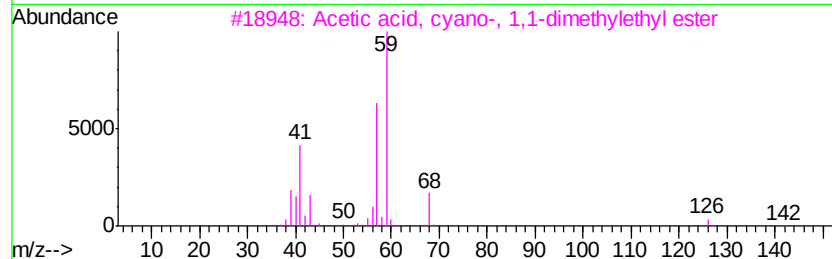
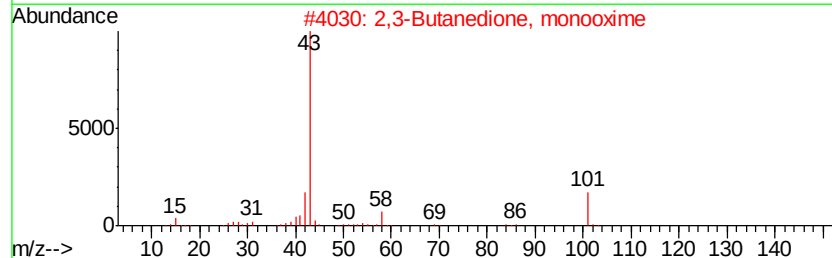
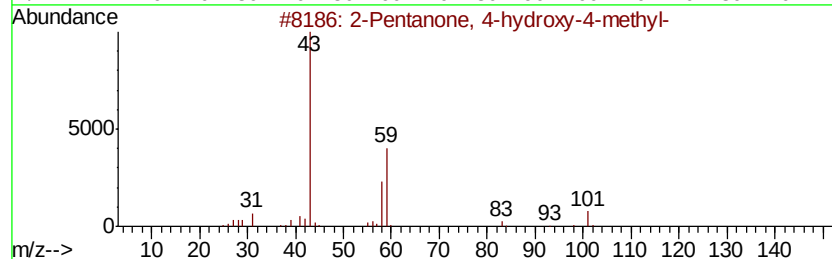
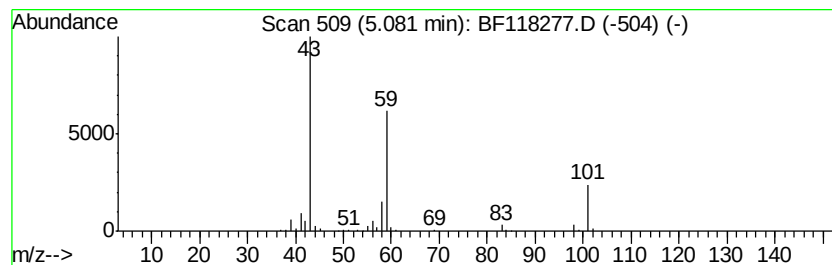
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	16.74 ng	568010	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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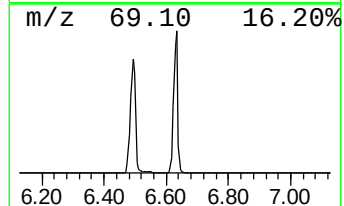
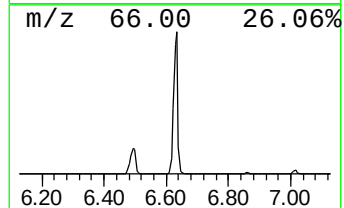
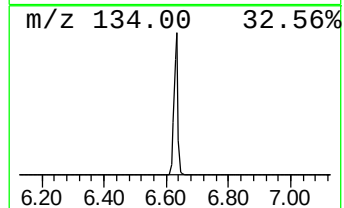
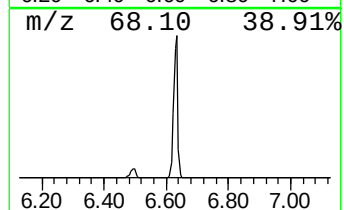
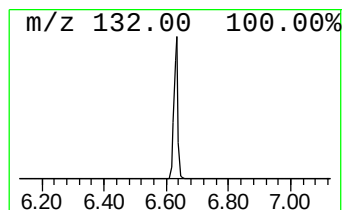
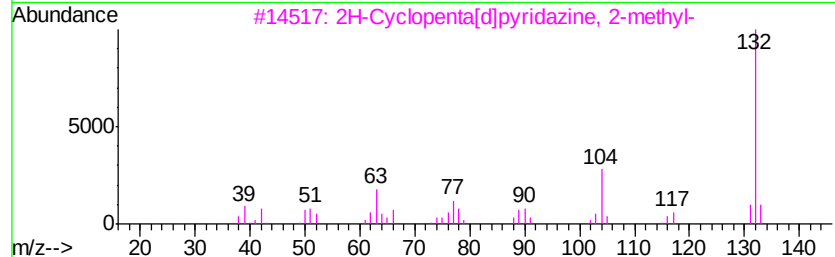
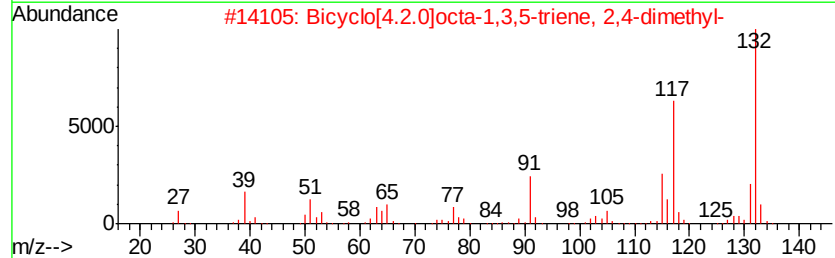
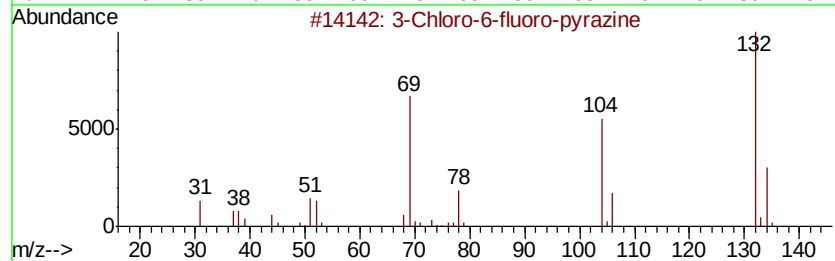
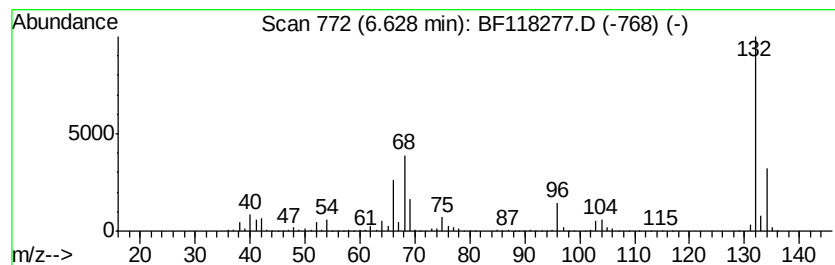
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	100.41 ng	3406620	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4		Xenon	132	Xe	007440-63-3	9
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9



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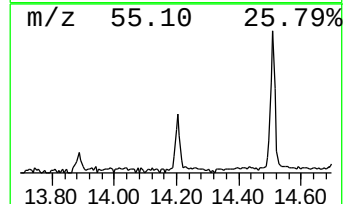
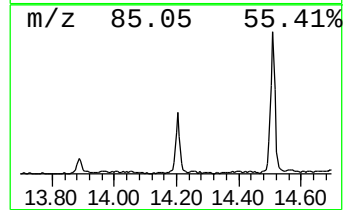
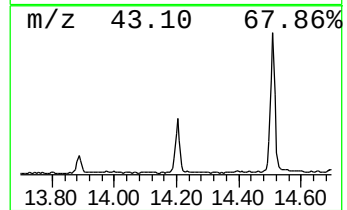
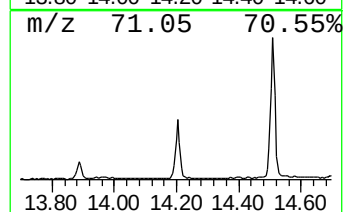
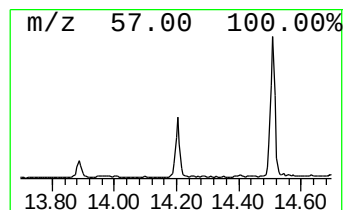
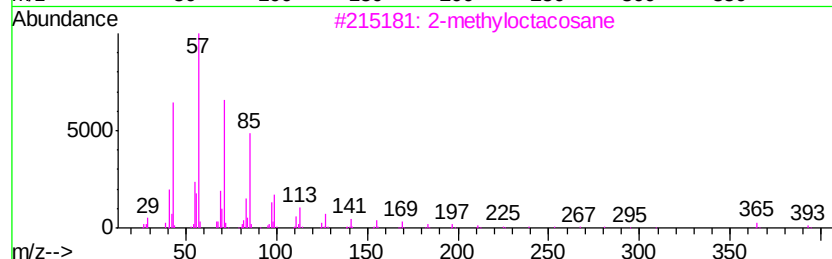
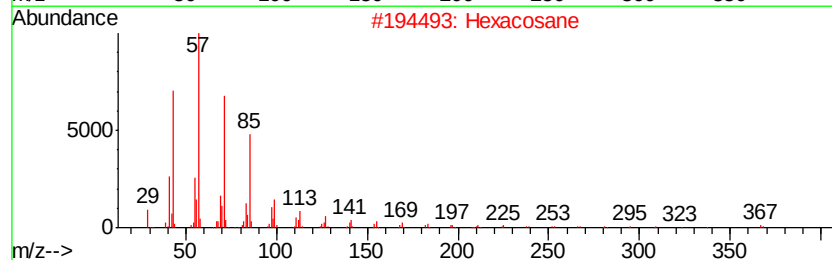
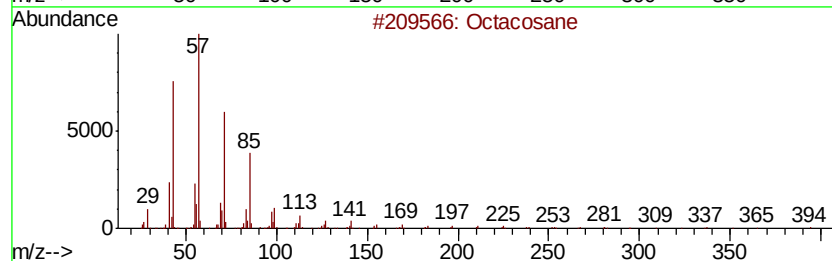
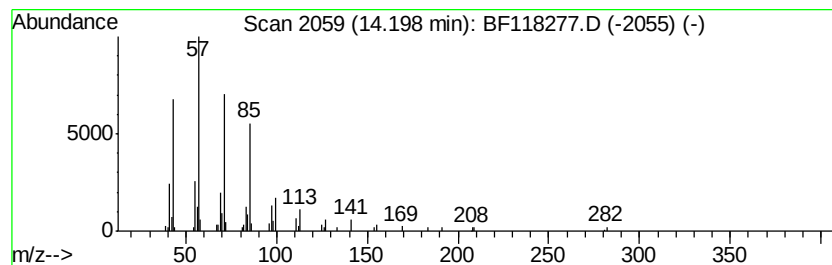
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 TIC Integration Parameters: LSCINT.P

 Peak Number 4 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.20	3.34 ng	137358	Chrysene-d12	14.05

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		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



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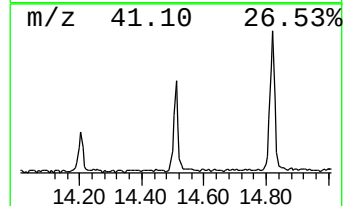
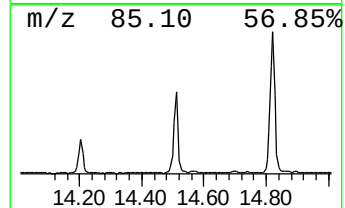
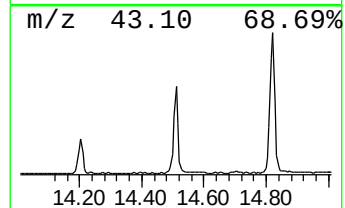
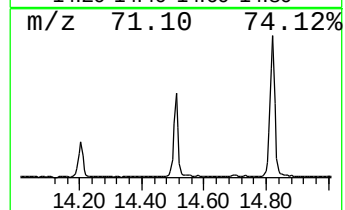
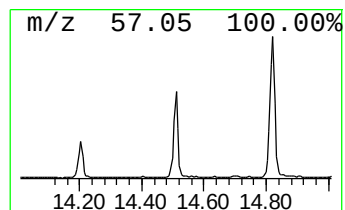
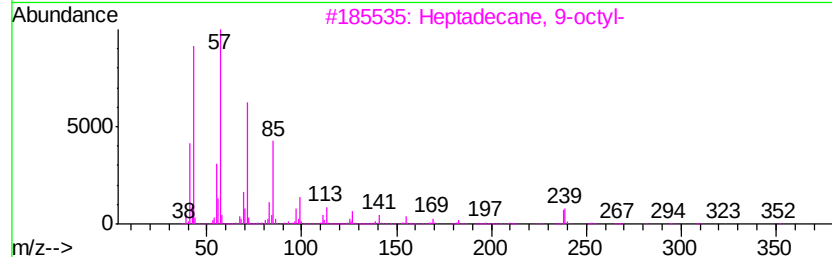
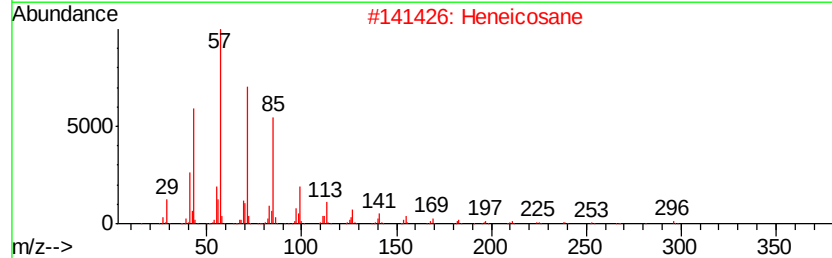
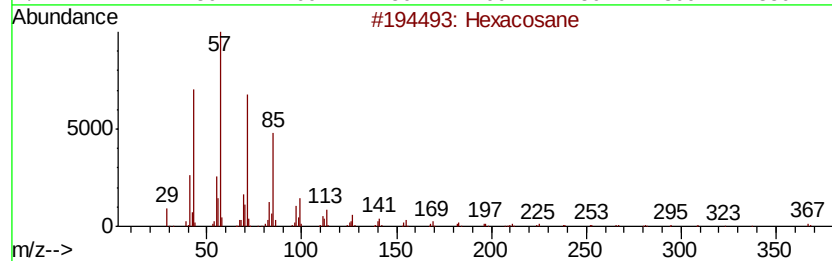
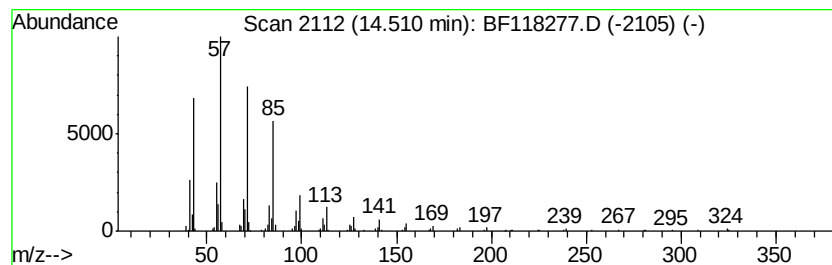
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	8.16 ng	335482	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Heptacosane	380	C27H56	000593-49-7	91
5		Heptadecane	240	C17H36	000629-78-7	91



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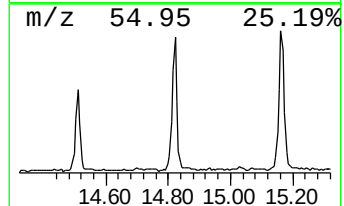
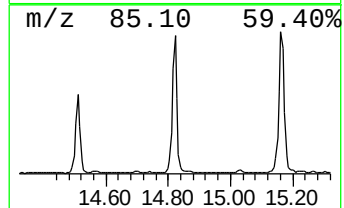
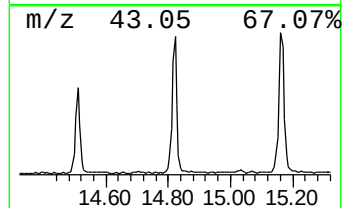
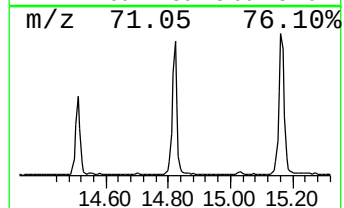
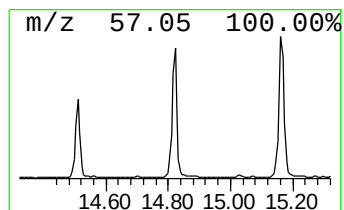
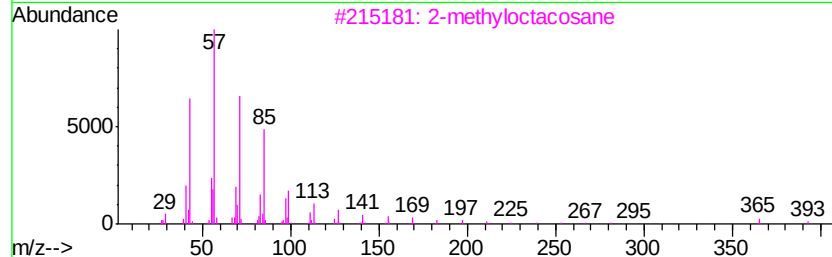
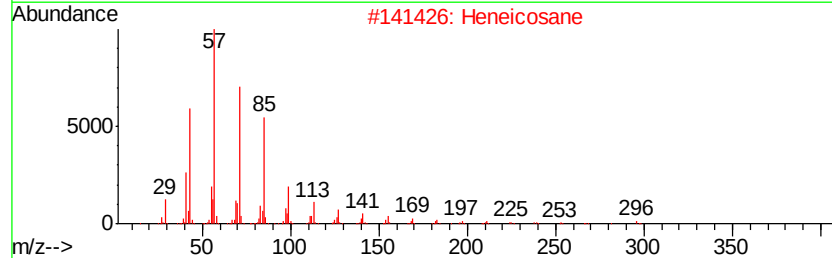
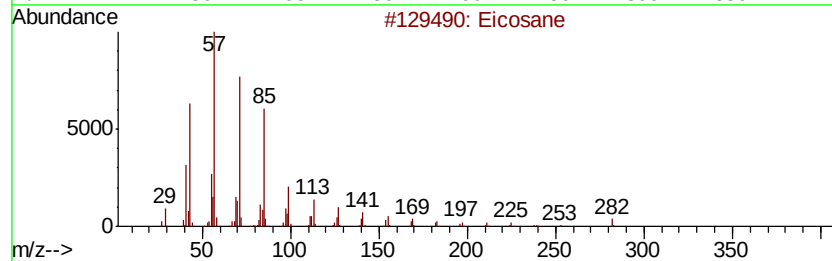
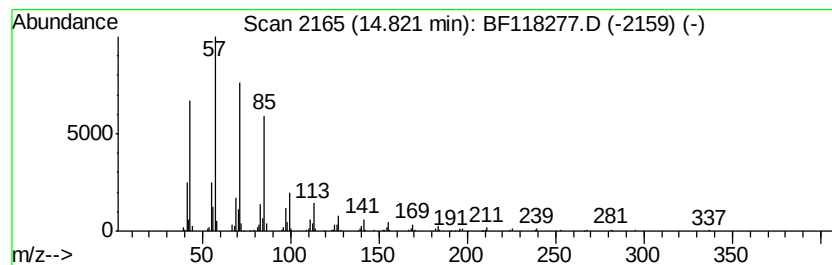
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	8.58 ng	603661	Perylene-d12	15.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	97
2	Heneicosane		296	C21H44	000629-94-7	91
3	2-methyloctacosane		408	C29H60	1000376-72-8	91
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
5	Docosane		310	C22H46	000629-97-0	91



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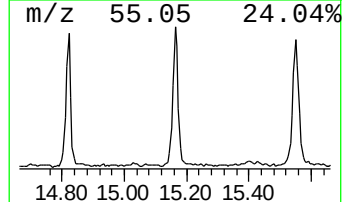
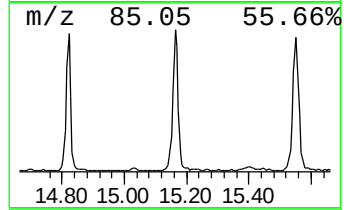
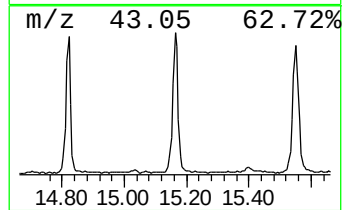
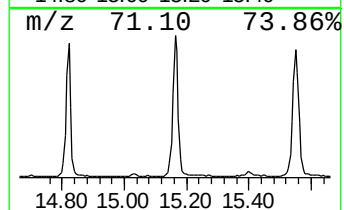
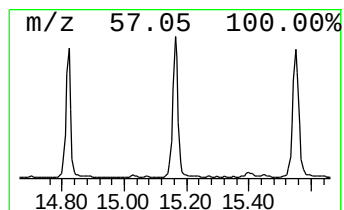
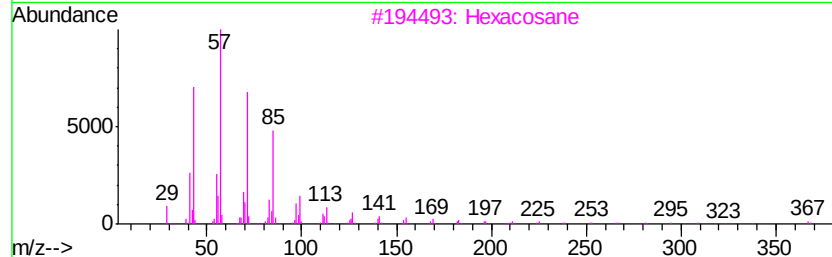
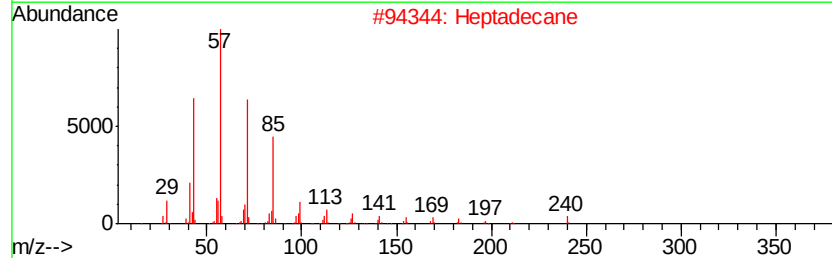
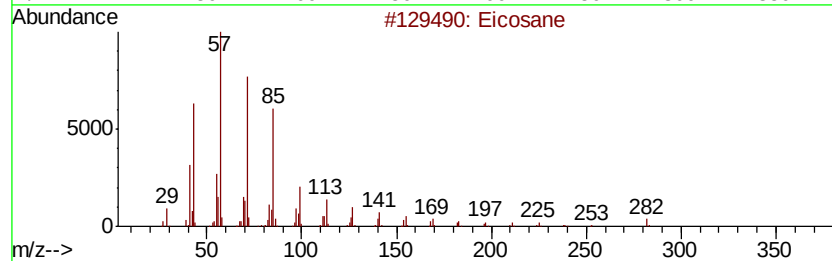
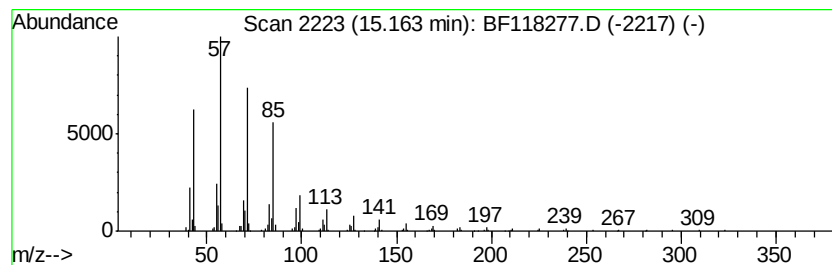
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.16	10.72 ng	753604	Perylene-d12		15.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	98
2	Heptadecane		240	C17H36	000629-78-7	95
3	Hexacosane		366	C26H54	000630-01-3	91
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
5	Heneicosane		296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\
Data File : BF118277.D
Acq On : 19 Dec 2019 14:10
Operator : JU
Sample : PB125579BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB125579BL

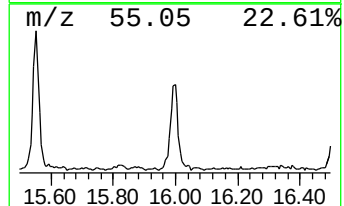
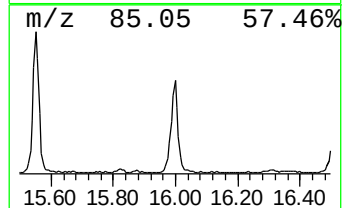
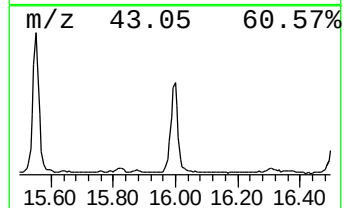
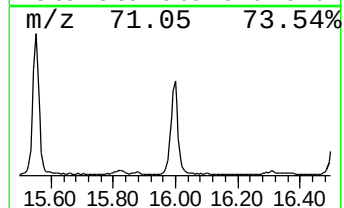
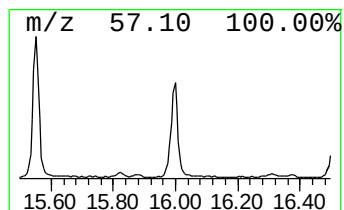
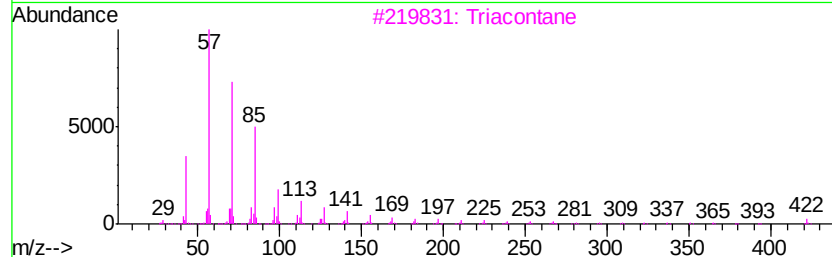
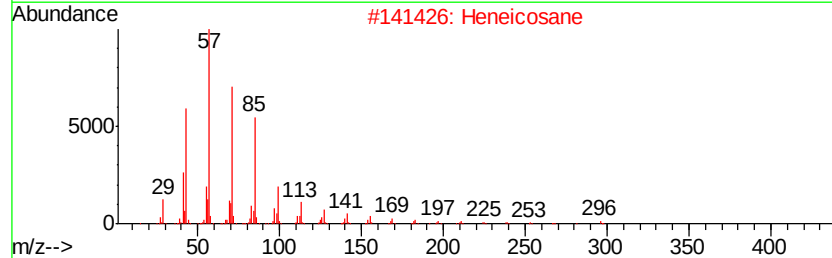
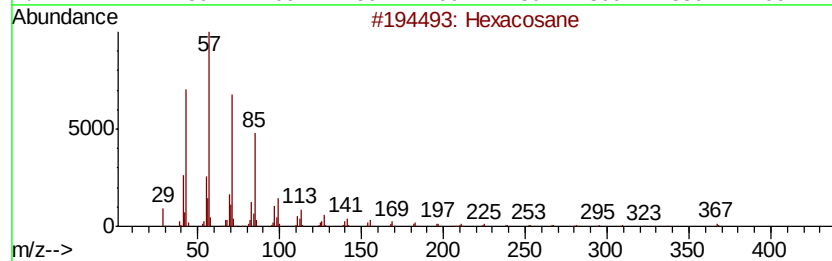
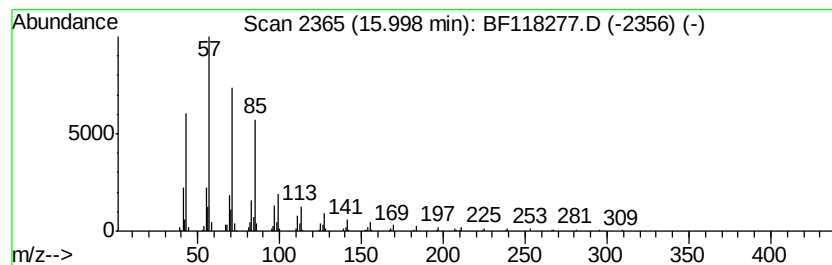
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	8.58 ng	603523	Perylene-d12	15.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	Triacontane		422	C30H62	000638-68-6	91
4	2-methyloctacosane		408	C29H60	1000376-72-8	91
5	Docosane		310	C22H46	000629-97-0	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\
Data File : BF118277.D
Acq On : 19 Dec 2019 14:10
Operator : JU
Sample : PB125579BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB125579BL

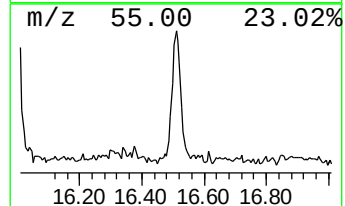
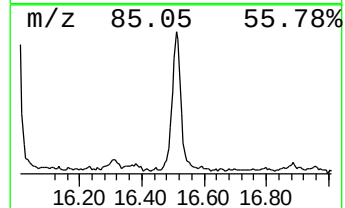
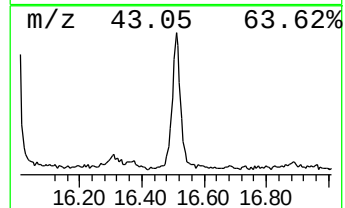
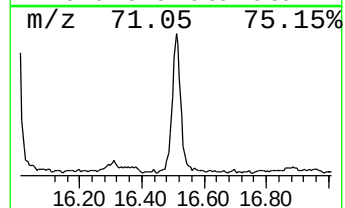
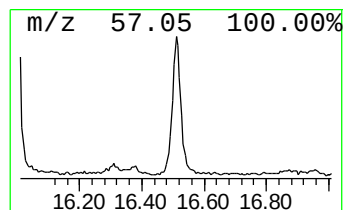
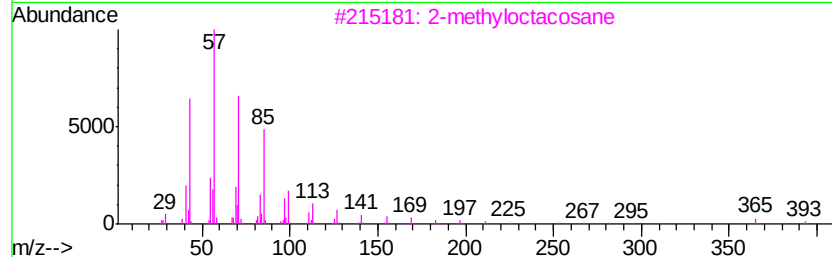
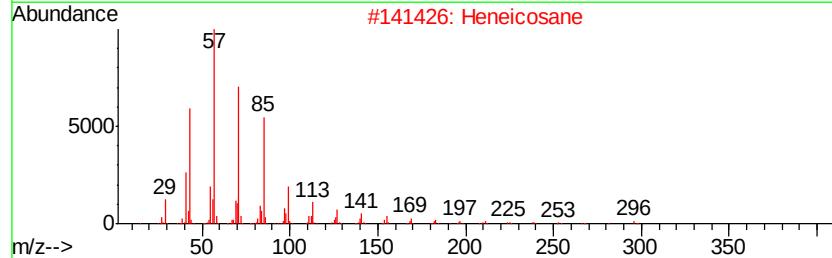
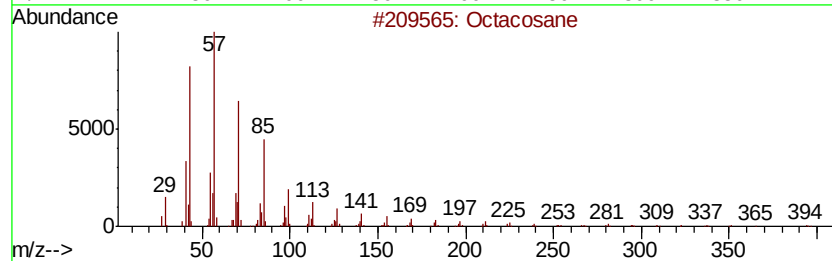
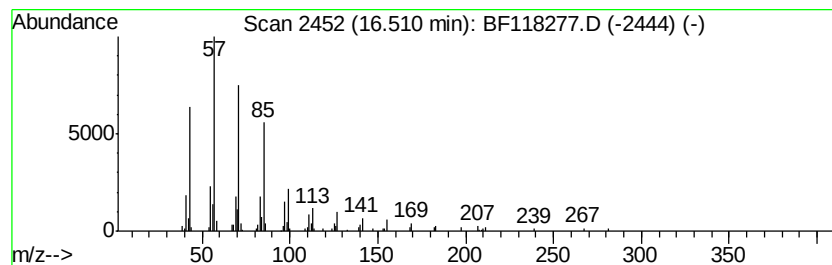
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.51	4.59 ng	322716	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Heptacosane	380	C27H56	000593-49-7	91
5		Pentacosane	352	C25H52	000629-99-2	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121919\
Data File : BF118277.D
Acq On : 19 Dec 2019 14:10
Operator : JU
Sample : PB125579BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB125579BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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...	5.08	16.7	ng	568010	1	6.86	678579	20.0
unknown6.63	6.63	100.4	ng	3406620	1	6.86	678579	20.0
Octacosane	14.20	3.3	ng	137358	5	14.05	822522	20.0
Hexacosane	14.51	8.2	ng	335482	5	14.05	822522	20.0
Eicosane	14.82	8.6	ng	603661	6	15.54	1406620	20.0
Heptadecane	15.16	10.7	ng	753604	6	15.54	1406620	20.0
Heneicosane	16.00	8.6	ng	603523	6	15.54	1406620	20.0
2-methyloctacosane	16.51	4.6	ng	322716	6	15.54	1406620	20.0