

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110118\
 Data File : BF110365.D
 Acq On : 1 Nov 2018 13:39
 Operator : JU/SJ
 Sample : J5741-35
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-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-BF102318.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	2.293	28	35	45	rVB	382558	500534	19.29%	2.434%
2	3.587	253	255	267	rBV	20300	44453	1.71%	0.216%
3	5.204	526	530	537	rBV	75415	101561	3.91%	0.494%
4	5.587	590	595	598	rBV	2187671	2170684	83.64%	10.557%
5	6.587	759	765	777	rBV	2024133	2412834	92.98%	11.735%
6	6.728	784	789	792	rBV	2526227	2349749	90.54%	11.428%
7	6.957	824	828	831	rBV	510501	443604	17.09%	2.157%
8	7.110	850	854	858	rBV	1943043	1792607	69.08%	8.718%
9	7.522	918	924	927	rBV	1407878	1449073	55.84%	7.047%
10	8.239	1041	1046	1062	rBV	600451	580001	22.35%	2.821%
11	9.310	1223	1228	1232	rBV	2747838	2595138	100.00%	12.621%
12	9.704	1291	1295	1304	rVB	276856	260361	10.03%	1.266%
13	9.998	1341	1345	1352	rBV	707916	626368	24.14%	3.046%
14	10.786	1475	1479	1492	rBV	1382046	1428930	55.06%	6.949%
15	11.486	1595	1598	1607	rBV	596576	562487	21.67%	2.736%
16	13.068	1863	1867	1870	rBV	1973325	1770878	68.24%	8.613%
17	13.945	2012	2016	2022	rBV	95468	118256	4.56%	0.575%
18	14.133	2044	2048	2055	rBV	427138	397182	15.30%	1.932%
19	14.263	2064	2070	2075	rBV	48539	76124	2.93%	0.370%
20	14.568	2119	2122	2130	rBV	43518	48588	1.87%	0.236%
21	14.886	2172	2176	2182	rBV	56004	61386	2.37%	0.299%
22	15.239	2231	2236	2239	rBV	62727	74287	2.86%	0.361%
23	15.657	2299	2307	2319	rVB2	327303	557411	21.48%	2.711%
24	16.092	2375	2381	2386	rBV	53492	83588	3.22%	0.407%
25	16.621	2466	2471	2479	rVB4	29750	55561	2.14%	0.270%

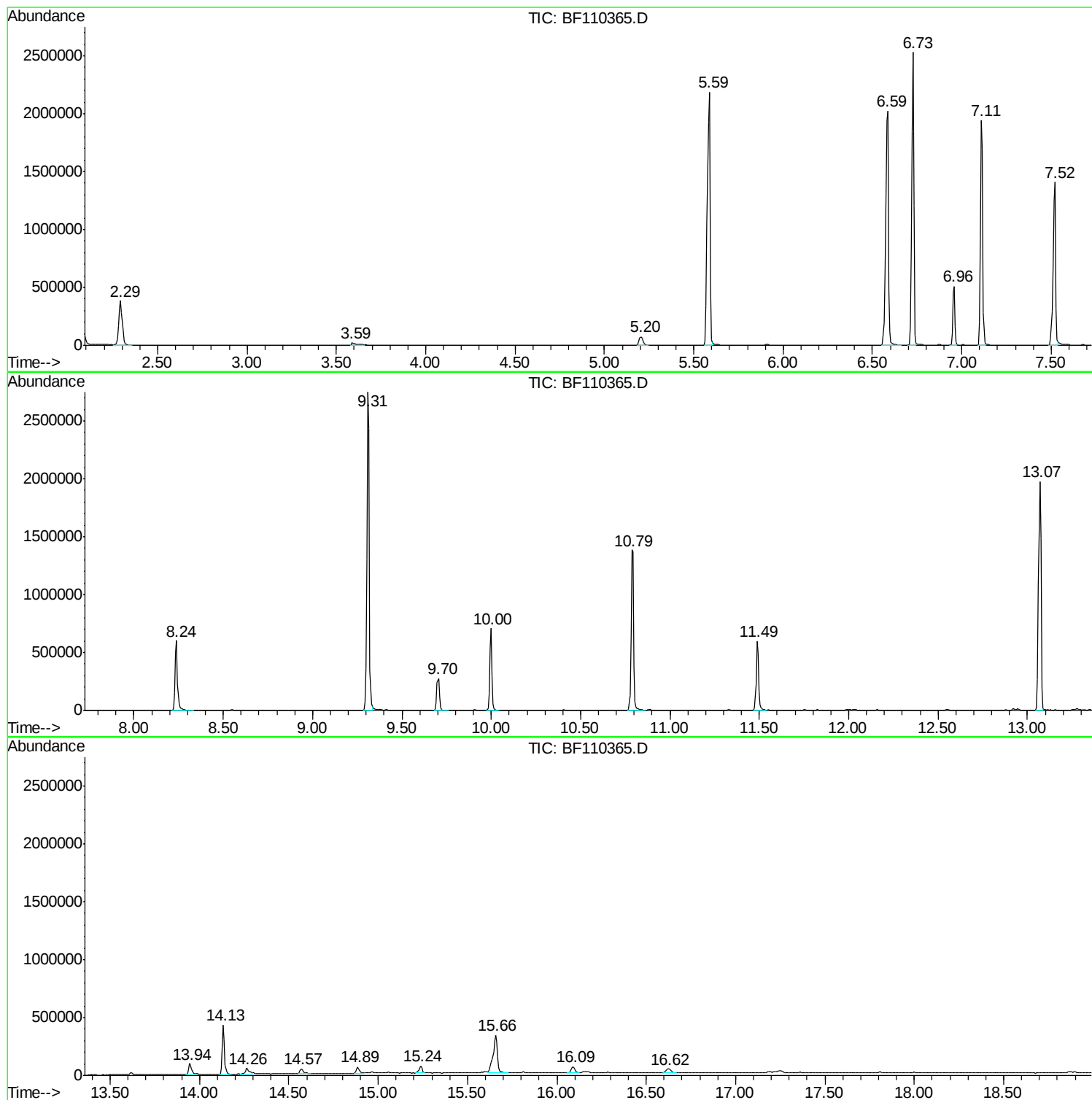
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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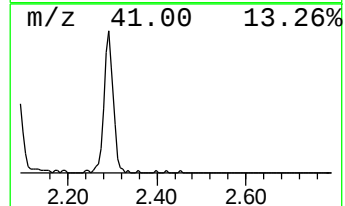
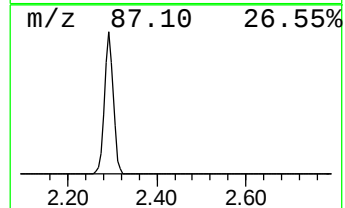
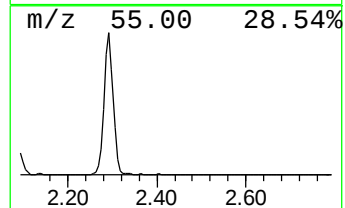
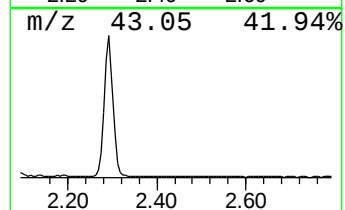
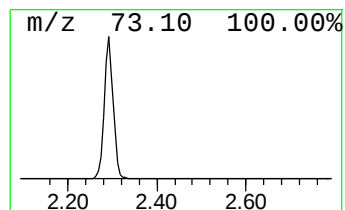
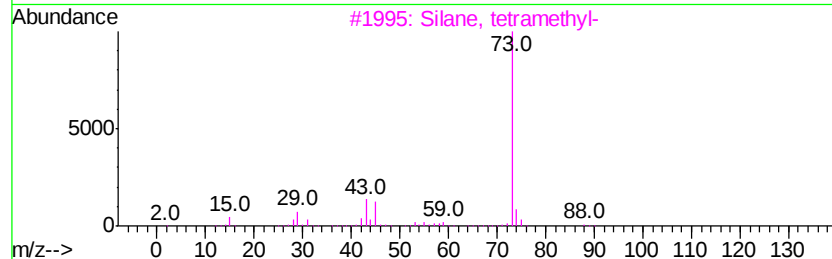
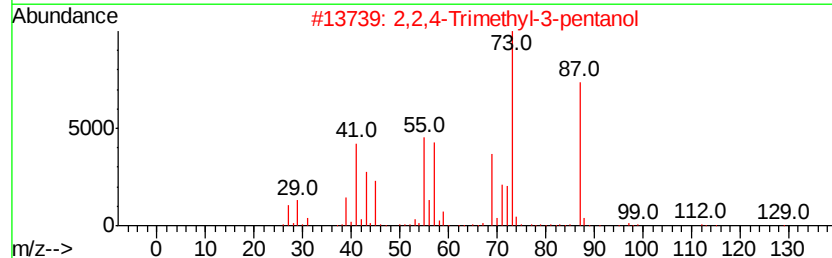
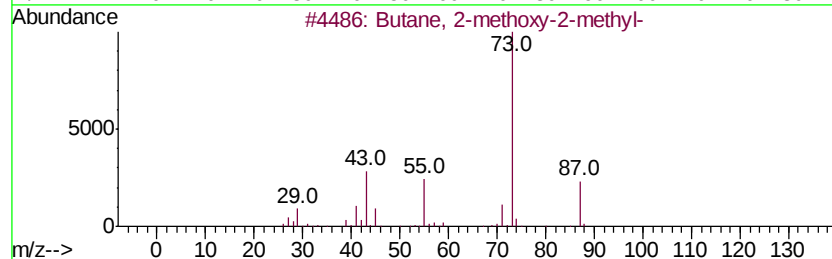
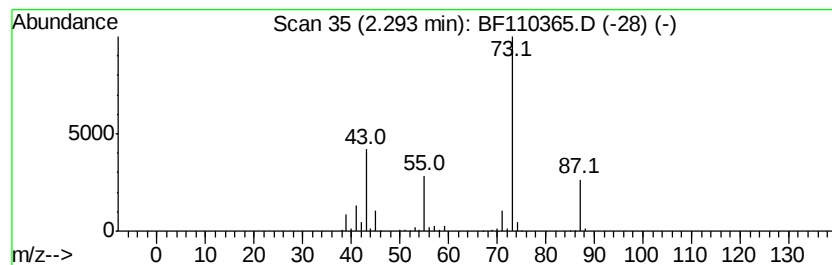
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.29	22.57 ng	500534	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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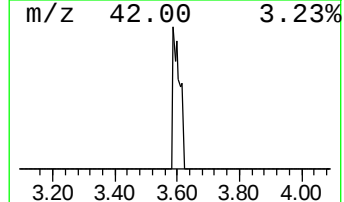
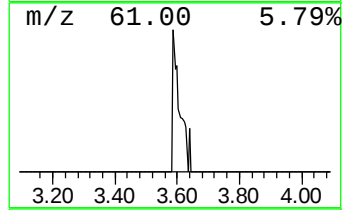
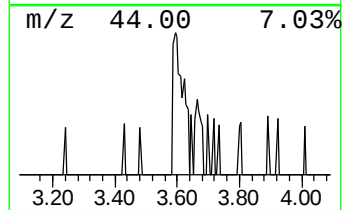
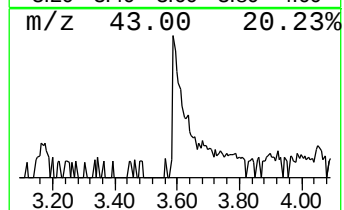
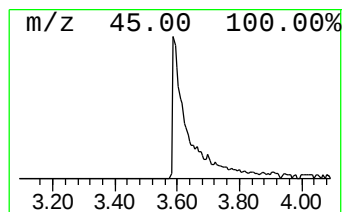
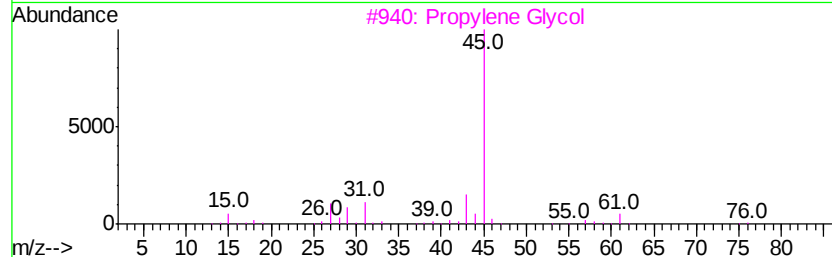
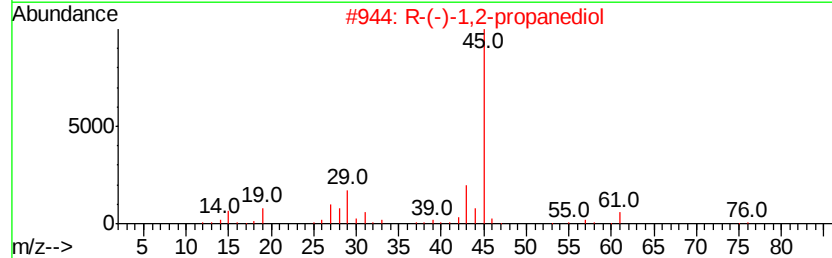
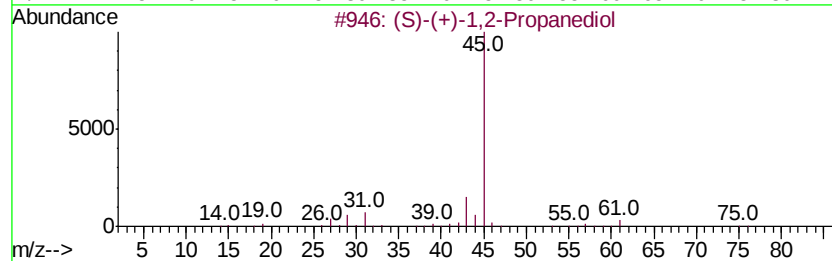
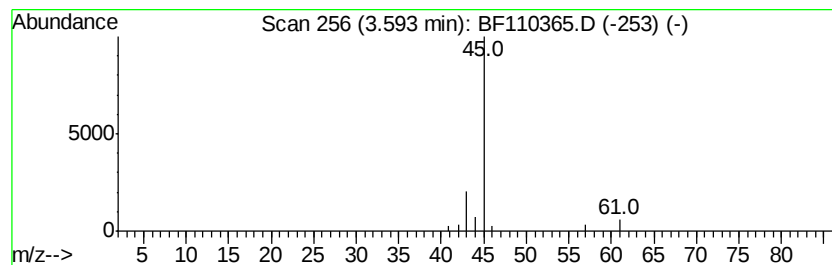
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.59	2.00 ng	44453	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3		Propylene Glycol	76	C3H8O2	000057-55-6	9
4		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5		Formamide	45	CH3NO	000075-12-7	5



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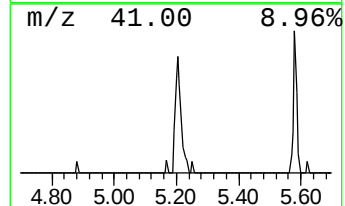
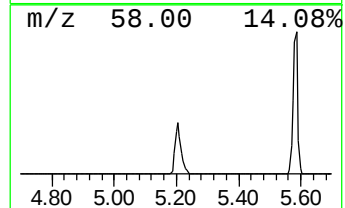
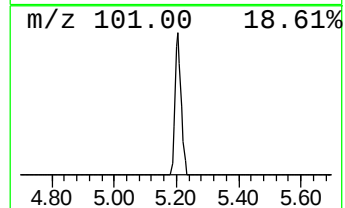
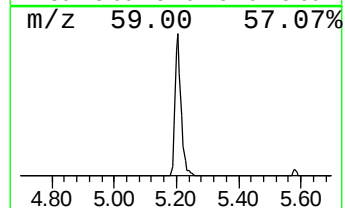
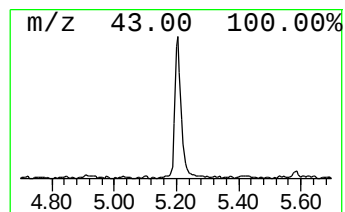
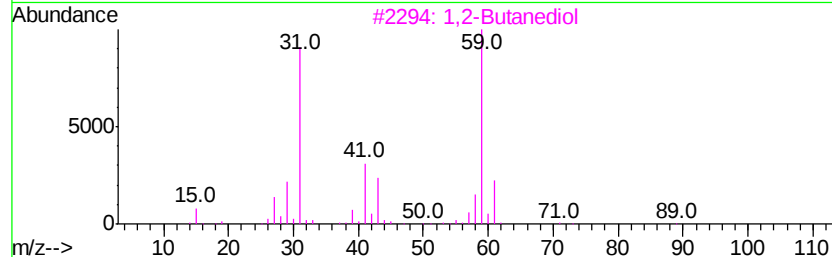
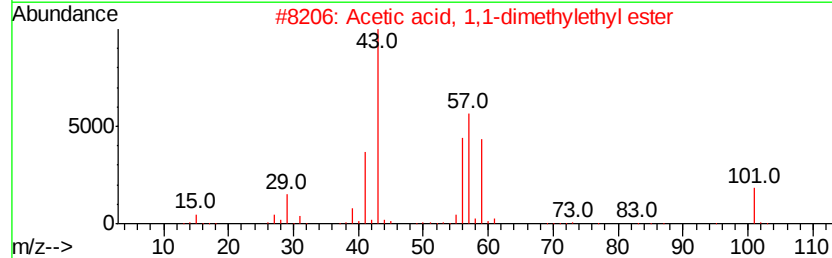
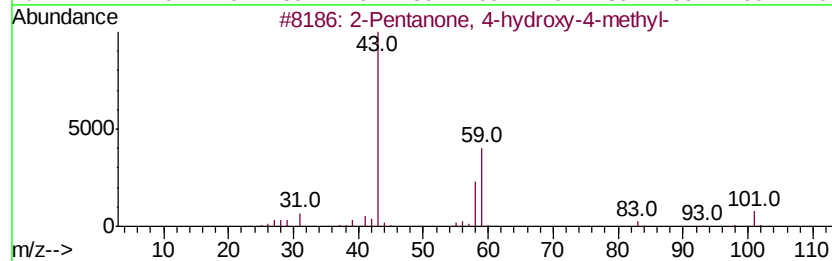
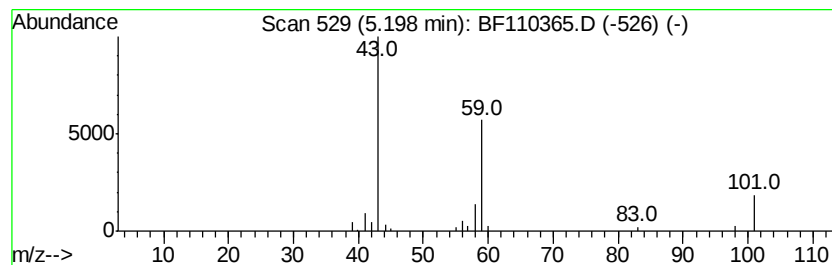
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	4.58 ng	101561	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		1,2-Butanediol	90	C4H10O2	000584-03-2	23
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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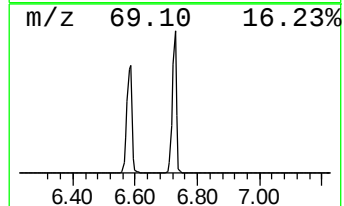
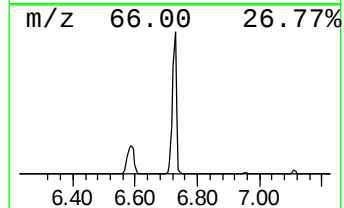
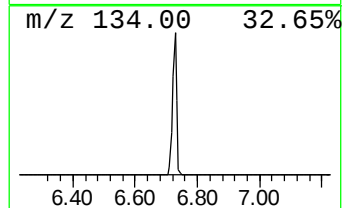
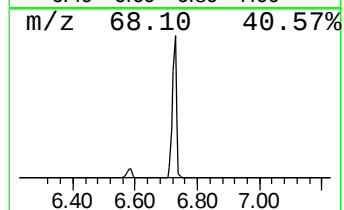
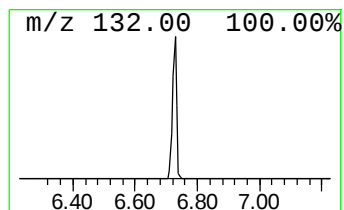
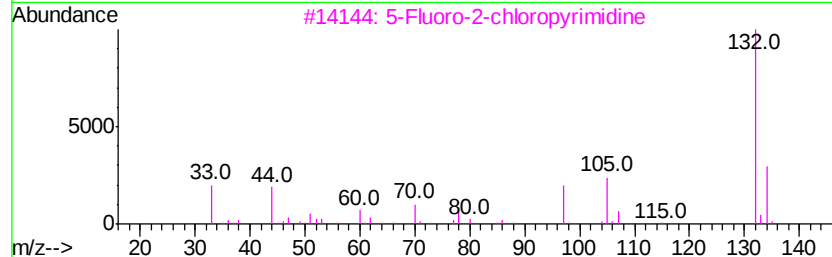
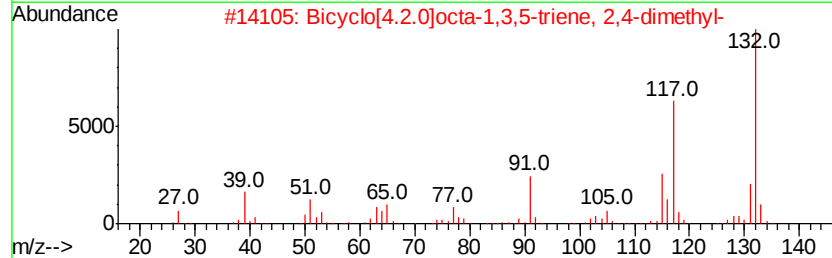
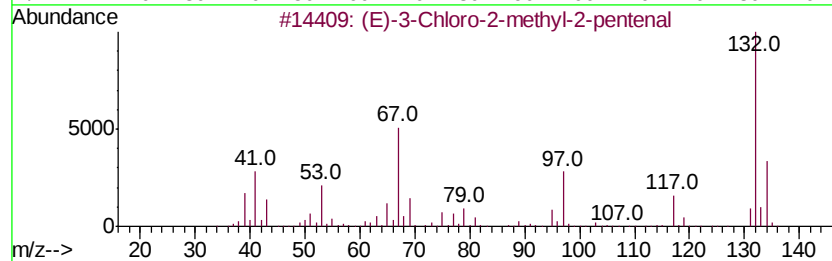
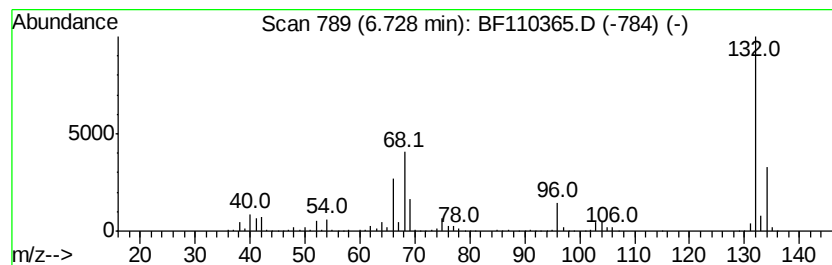
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	105.94 ng	2349750	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		Xenon	132	Xe	007440-63-3	9



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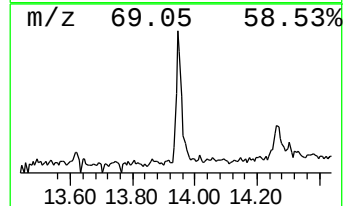
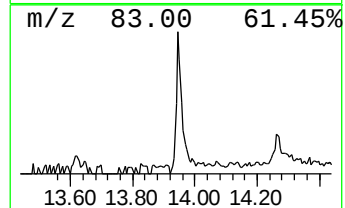
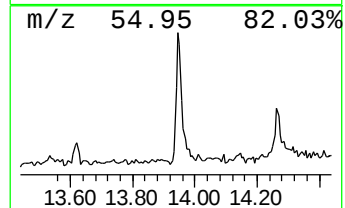
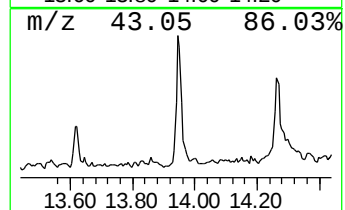
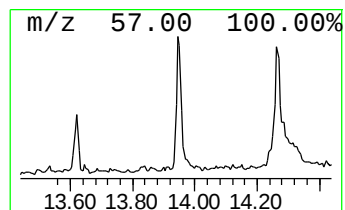
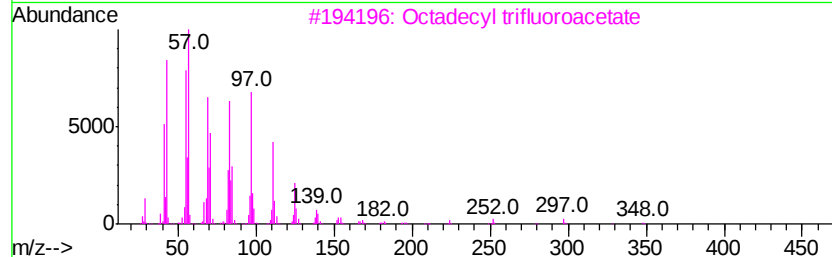
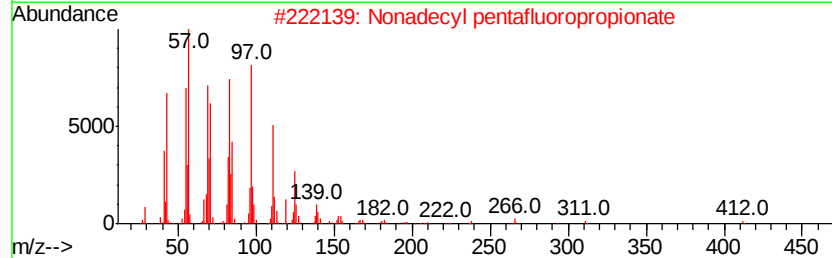
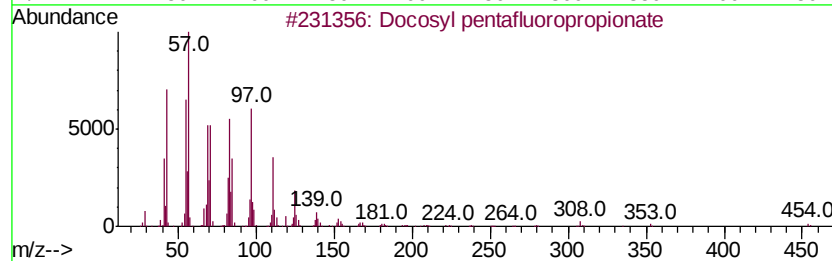
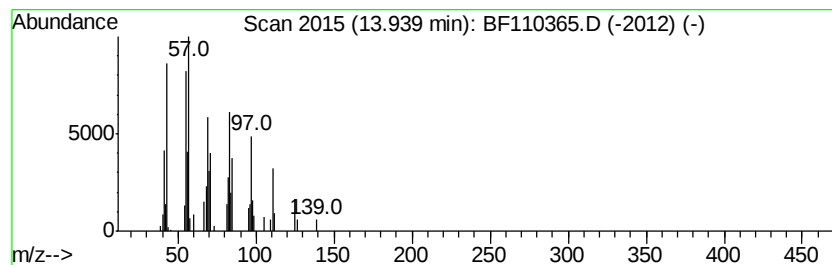
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Docosyl pentafluoropropionate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	5.95 ng	118256	Chrysene-d12	14.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
2		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	87
4		17-Pentatriacontene	491	C35H70	006971-40-0	83
5		1-Heneicosanol	312	C21H44O	015594-90-8	76



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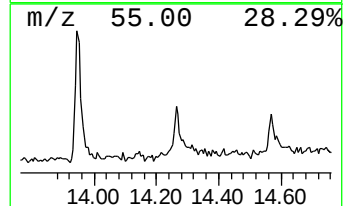
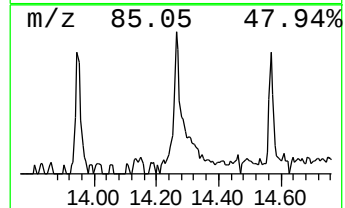
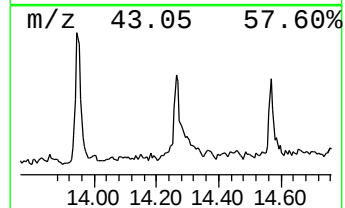
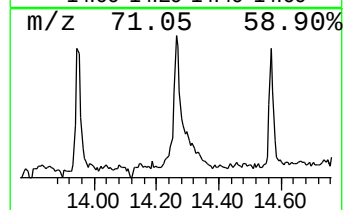
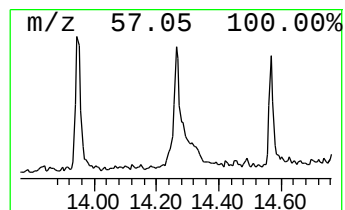
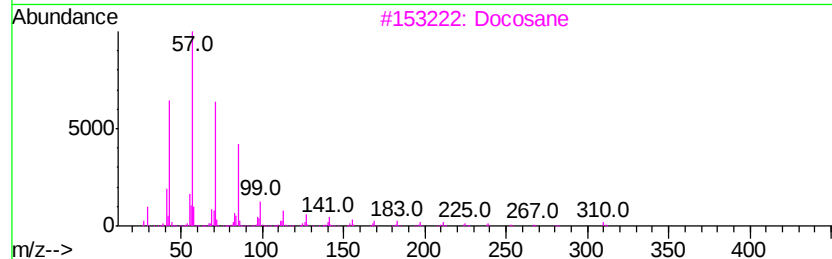
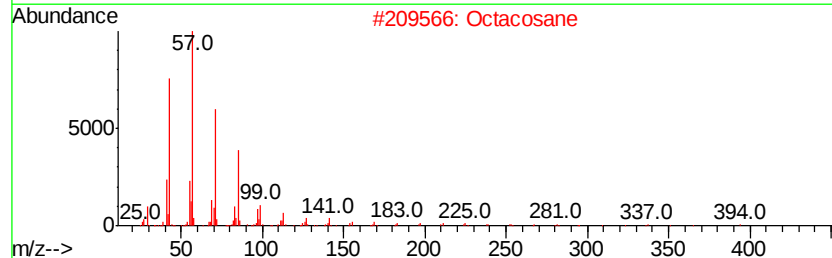
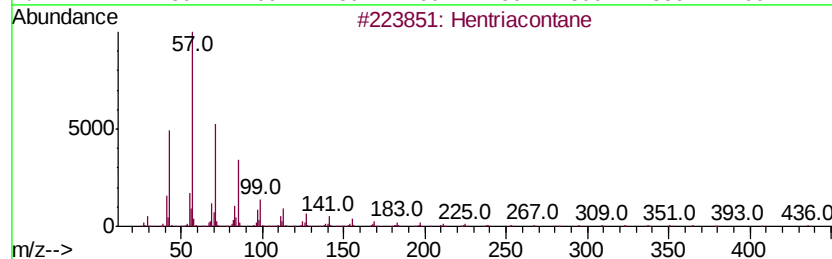
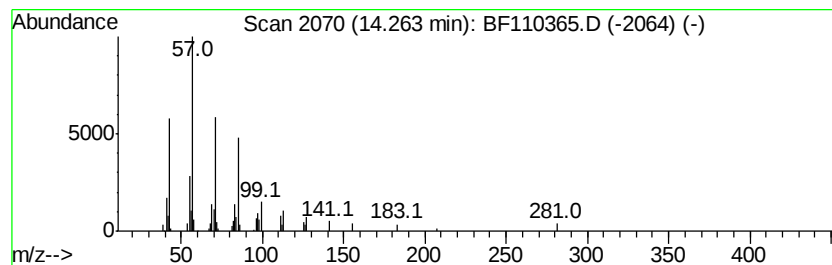
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	3.83 ng	76124	Chrysene-d12	14.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	91
2	Octacosane		394	C28H58	000630-02-4	91
3	Docosane		310	C22H46	000629-97-0	90
4	Hexacosane		366	C26H54	000630-01-3	87
5	Heneicosane		296	C21H44	000629-94-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110365.D
Acq On : 1 Nov 2018 13:39
Operator : JU/SJ
Sample : J5741-35
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-9

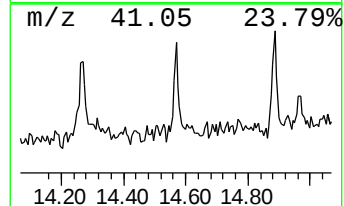
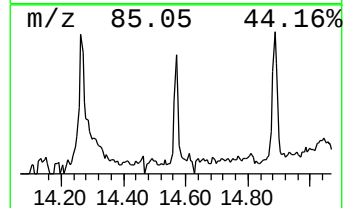
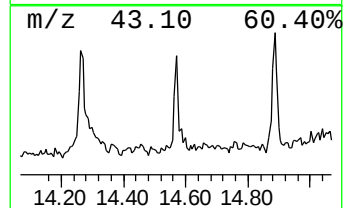
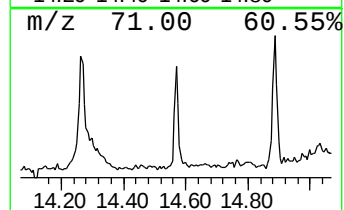
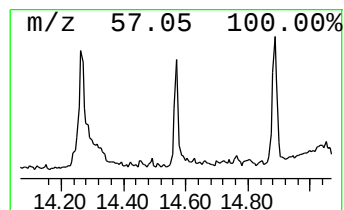
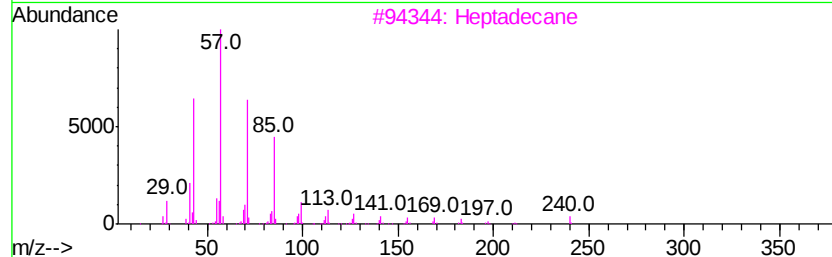
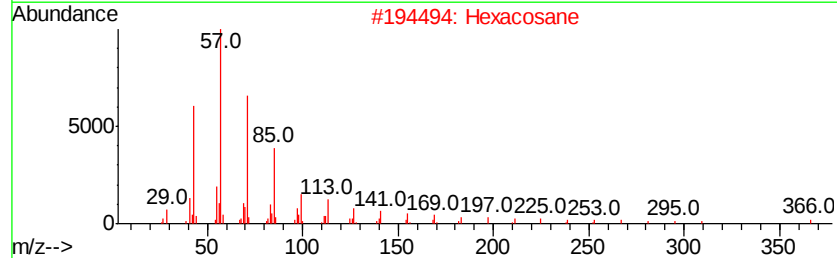
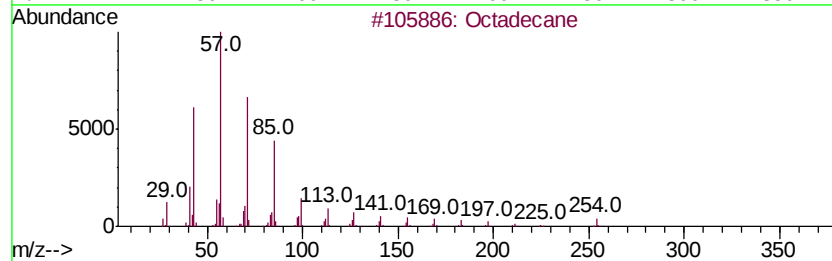
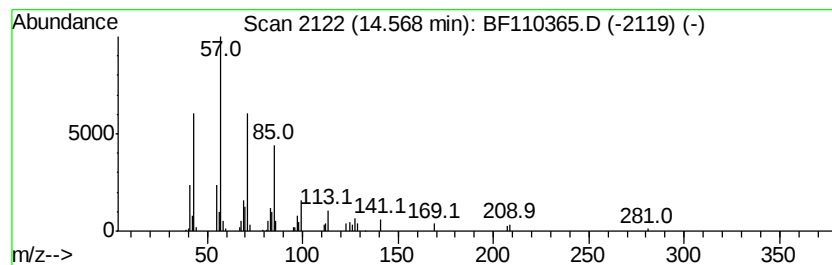
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	2.45 ng	48588	Chrysene-d12	14.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	91
2		Hexacosane	366	C26H54	000630-01-3	90
3		Heptadecane	240	C17H36	000629-78-7	90
4		Hexadecane	226	C16H34	000544-76-3	90
5		Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110365.D
Acq On : 1 Nov 2018 13:39
Operator : JU/SJ
Sample : J5741-35
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-9

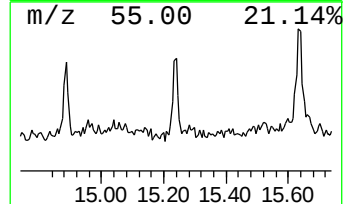
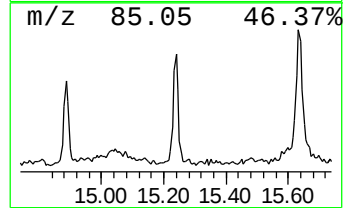
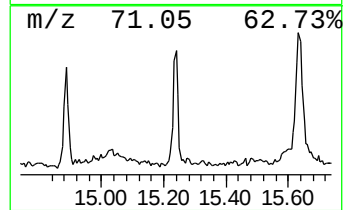
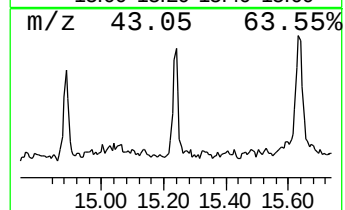
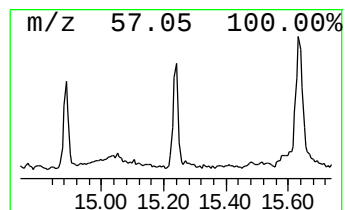
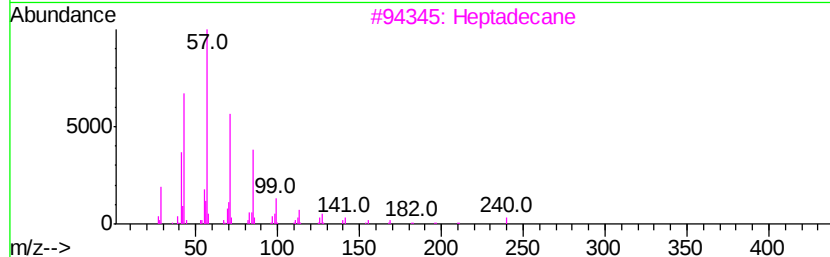
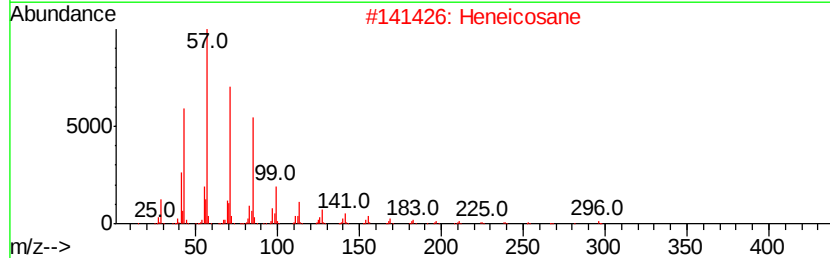
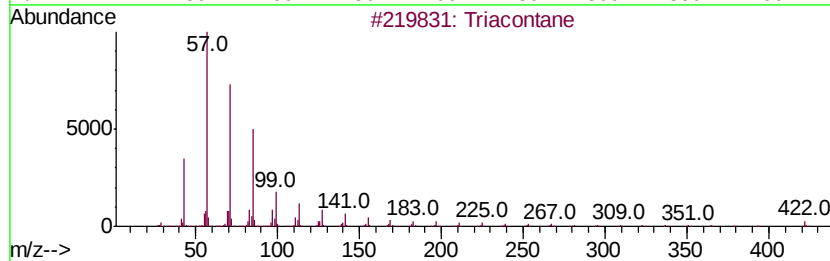
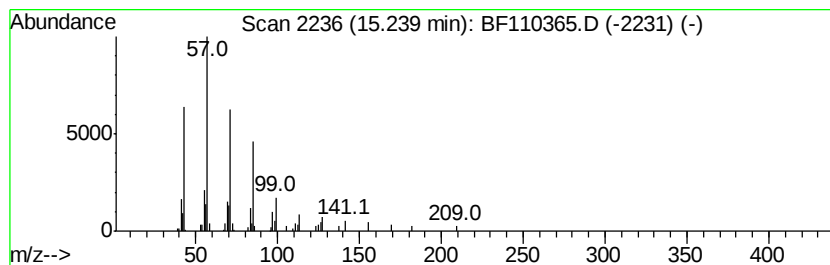
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Triacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	2.67 ng	74287	Perylene-d12	15.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane	422	C30H62	000638-68-6	91
2			Heneicosane	296	C21H44	000629-94-7	90
3			Heptadecane	240	C17H36	000629-78-7	90
4			Docosane	310	C22H46	000629-97-0	90
5			Hentriacontane	437	C31H64	000630-04-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110365.D
Acq On : 1 Nov 2018 13:39
Operator : JU/SJ
Sample : J5741-35
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-9

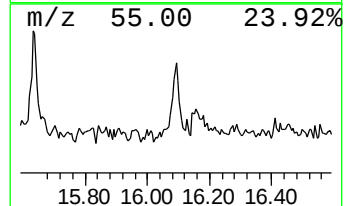
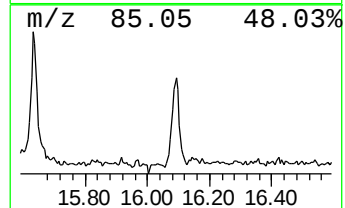
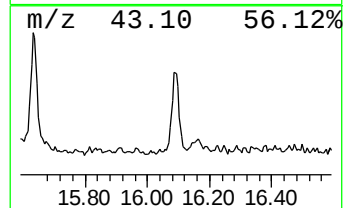
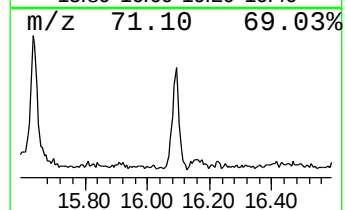
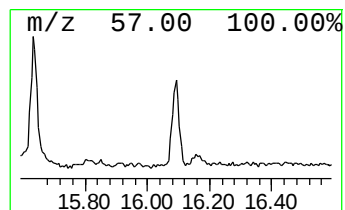
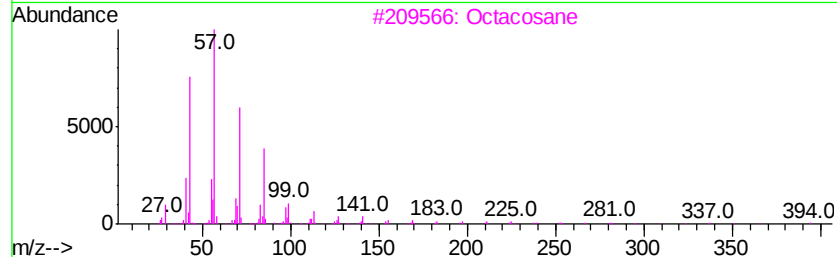
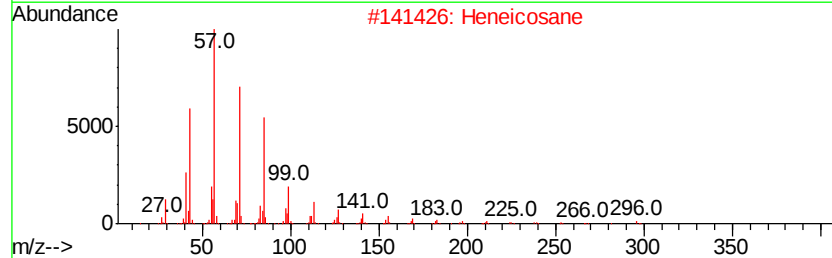
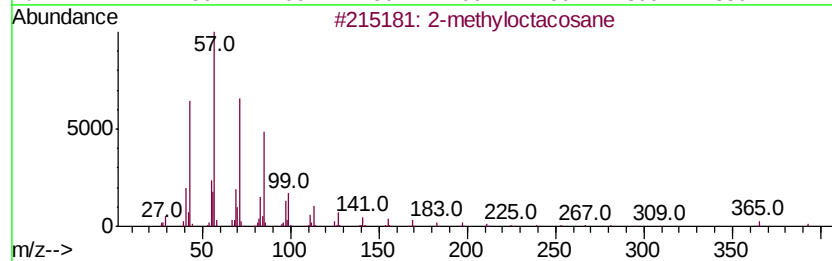
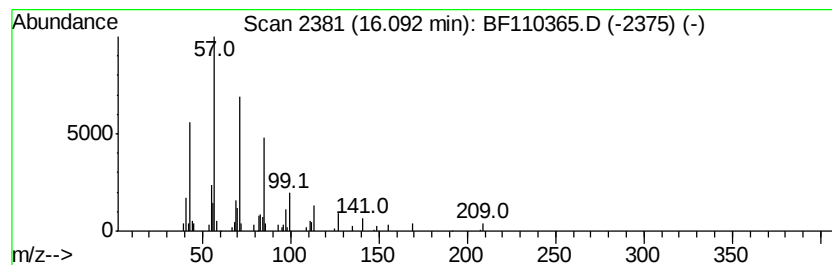
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.09	3.00 ng	83588	Perylene-d12	15.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Heneicosane	296	C21H44	000629-94-7	90
3		Octacosane	394	C28H58	000630-02-4	90
4		Heptadecane	240	C17H36	000629-78-7	87
5		Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110118\
Data File : BF110365.D
Acq On : 1 Nov 2018 13:39
Operator : JU/SJ
Sample : J5741-35
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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...	2.29	22.6	ng	500534	1	6.96	443604	20.0
(S)-(+)-1,2-Propa...	3.59	2.0	ng	44453	1	6.96	443604	20.0
2-Pentanone, 4-hy...	5.20	4.6	ng	101561	1	6.96	443604	20.0
unknown6.73	6.73	105.9	ng	2349750	1	6.96	443604	20.0
Docosyl pentaflu...	13.94	6.0	ng	118256	5	14.13	397182	20.0
Hentriacontane	14.26	3.8	ng	76124	5	14.13	397182	20.0
Octadecane	14.57	2.5	ng	48588	5	14.13	397182	20.0
Triacontane	15.24	2.7	ng	74287	6	15.66	557411	20.0
2-methyloctacosane	16.09	3.0	ng	83588	6	15.66	557411	20.0