

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070616\
 Data File : BF088752.D
 Acq On : 6 Jul 2016 23:56
 Operator : UM/SJ
 Sample : H3878-13
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C2.1-09

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:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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	1.701	8	10	19	rVB	195599	314892	9.38%	1.294%
2	1.827	19	21	68	rVB	1574306	3358636	100.00%	13.805%
3	4.913	289	291	296	rBB	79551	116375	3.46%	0.478%
4	5.336	325	328	331	rBV	1484150	2057051	61.25%	8.455%
5	6.387	416	420	422	rBV	1942833	2174243	64.74%	8.937%
6	6.513	428	431	434	rBV	2051639	2035423	60.60%	8.366%
7	6.742	449	451	453	rVB	438646	515049	15.34%	2.117%
8	6.902	463	465	467	rBB	1674173	1505838	44.83%	6.189%
9	7.313	498	501	503	rBV	1418602	1440497	42.89%	5.921%
10	8.033	561	564	566	rBV	845953	782541	23.30%	3.216%
11	8.650	616	618	620	rBB	178894	148389	4.42%	0.610%
12	9.108	655	658	661	rBV	2222899	2156424	64.21%	8.863%
13	9.508	690	693	695	rVB	245486	319564	9.51%	1.313%
14	9.782	714	717	719	rVV	922218	879827	26.20%	3.616%
15	10.228	752	756	757	rBV	48465	51729	1.54%	0.213%
16	10.559	783	785	788	rBV2	1086666	1395061	41.54%	5.734%
17	10.696	795	797	801	rBV	63657	73947	2.20%	0.304%
18	11.142	834	836	837	rBV	94822	81982	2.44%	0.337%
19	11.256	844	846	848	rVV	1030336	892017	26.56%	3.666%
20	11.325	848	852	856	rVB5	17468	47530	1.42%	0.195%
21	11.565	871	873	878	rVB	55265	50862	1.51%	0.209%
22	12.834	982	984	987	rBV	1641959	2279439	67.87%	9.369%
23	13.748	1061	1064	1073	rBV	133330	214686	6.39%	0.882%
24	13.874	1073	1075	1078	rBV	823083	741743	22.08%	3.049%
25	14.377	1114	1119	1125	rBV2	39879	86803	2.58%	0.357%
26	15.257	1193	1196	1199	rBV	470346	527272	15.70%	2.167%
27	16.731	1322	1325	1329	rBV	48234	81924	2.44%	0.337%

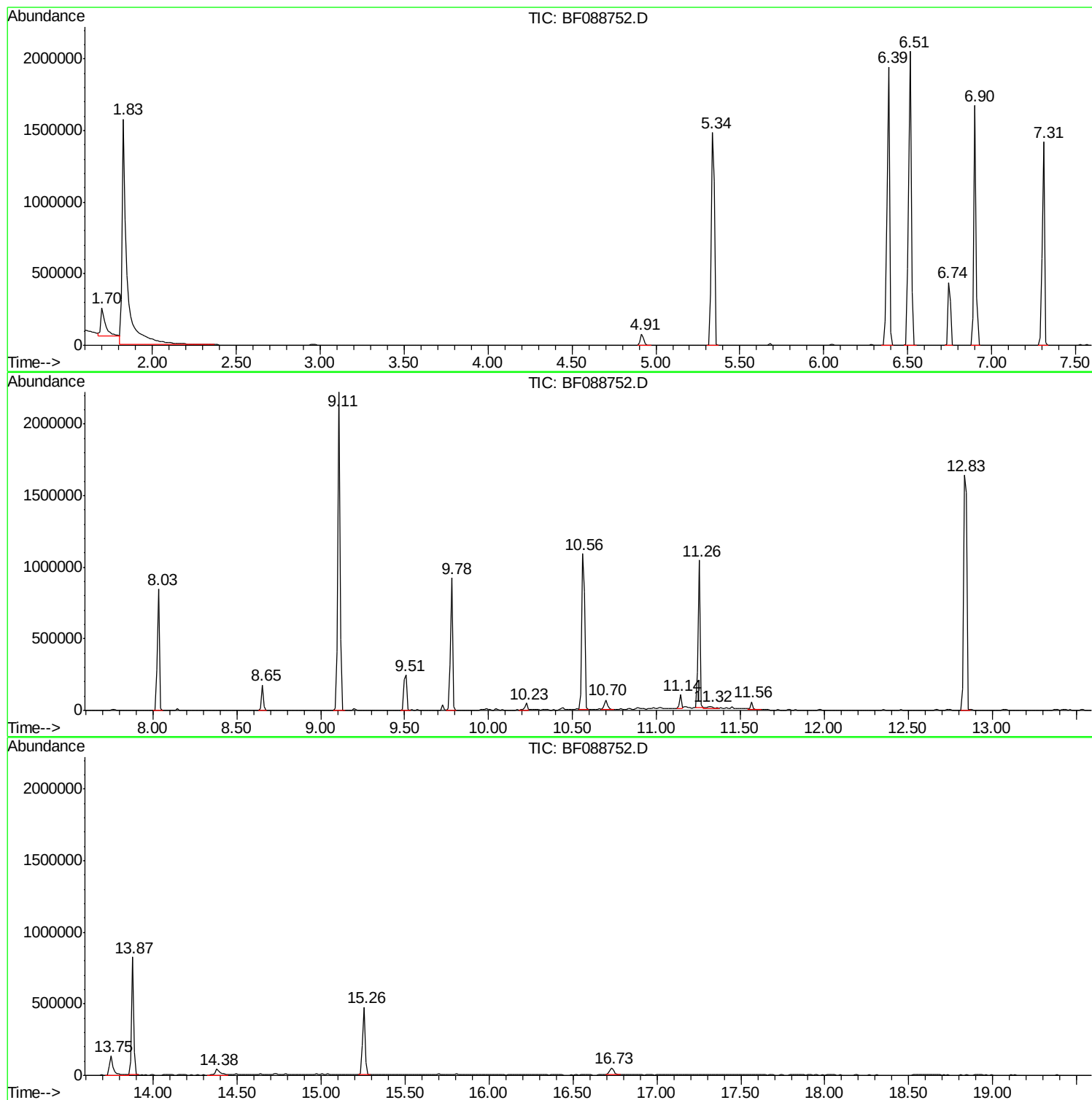
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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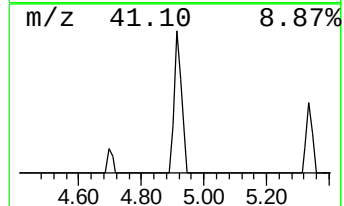
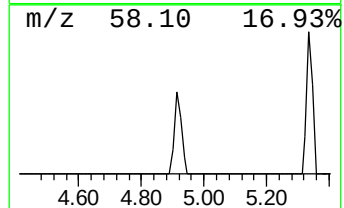
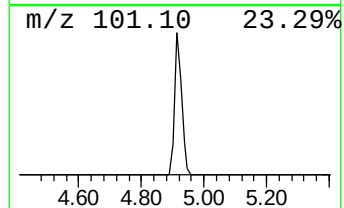
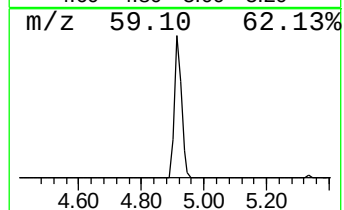
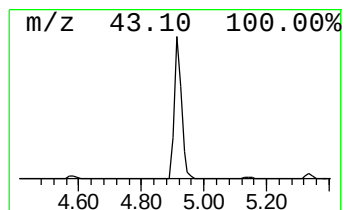
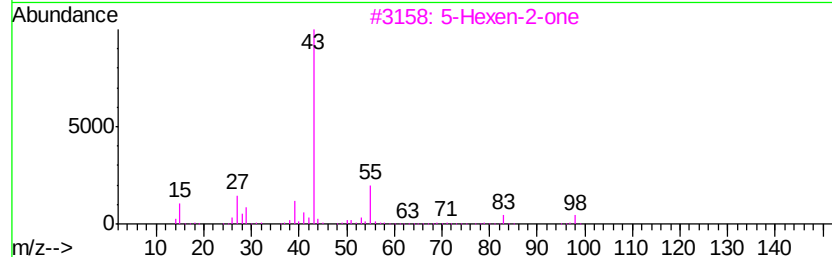
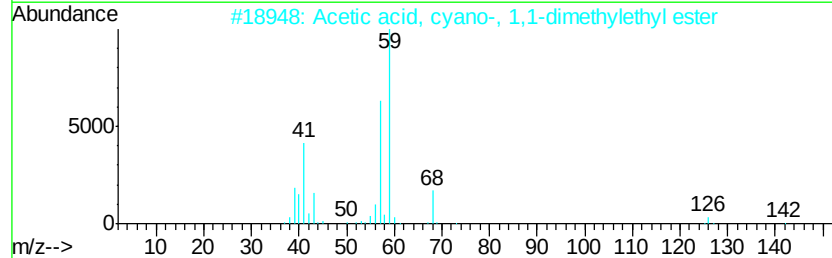
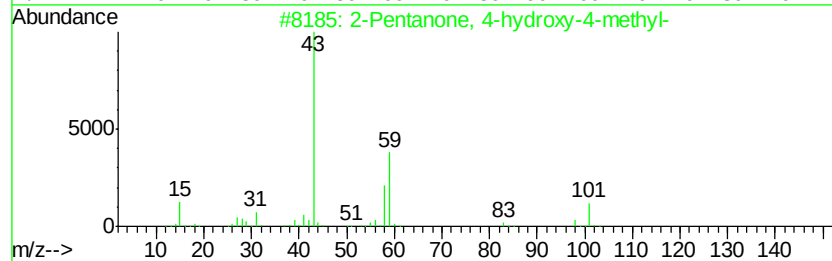
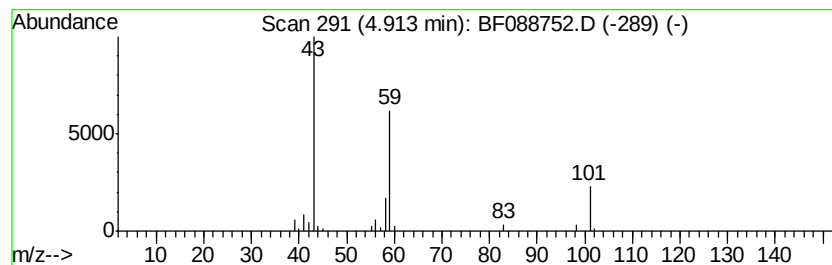
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	4.52 ng	116375	1,4-Dichlorobenzene-d4	6.74

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23	
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9	
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9	
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9	



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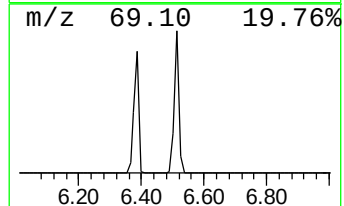
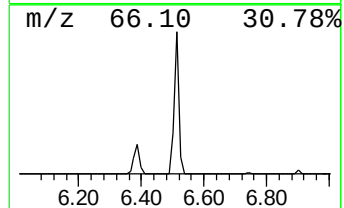
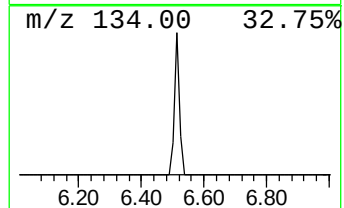
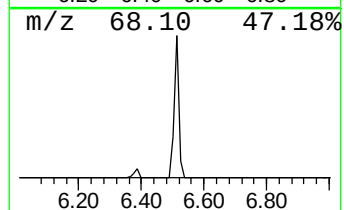
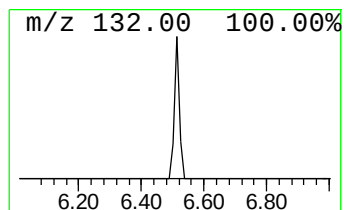
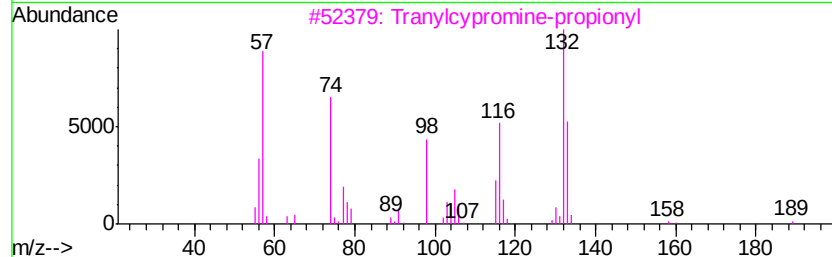
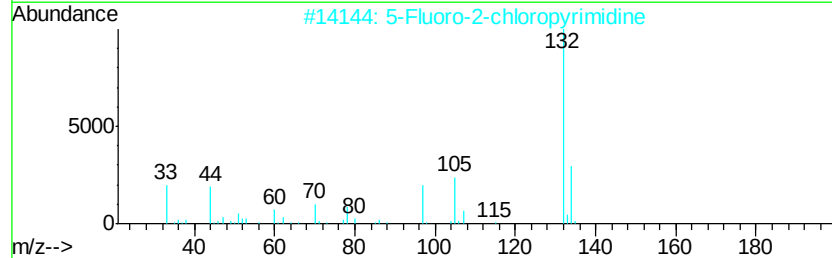
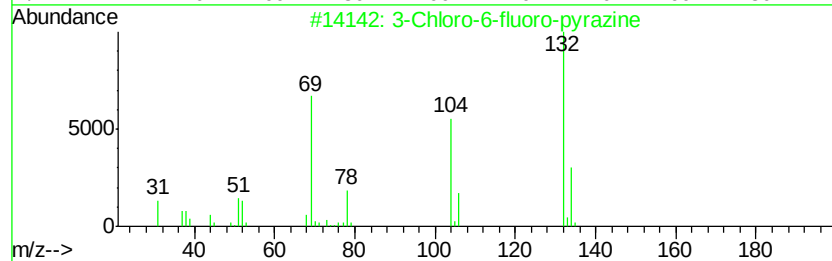
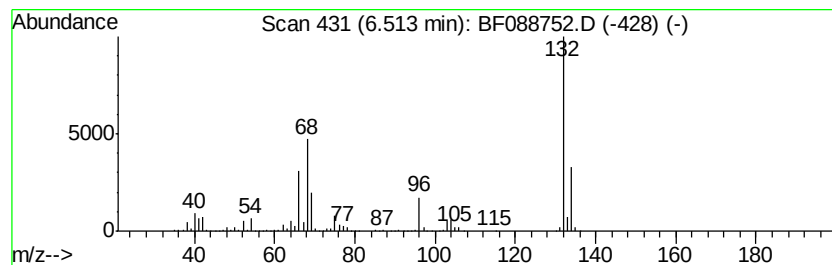
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Peak Number 4 unknown6.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	79.04 ng	2035420	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropamine-propionyl	189	C12H15NO	1000123-86-3	10
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5		N-(3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10



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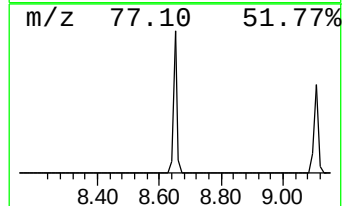
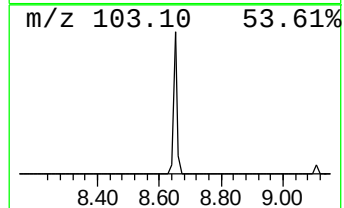
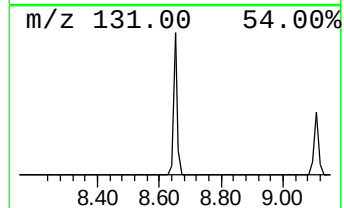
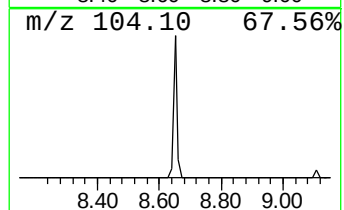
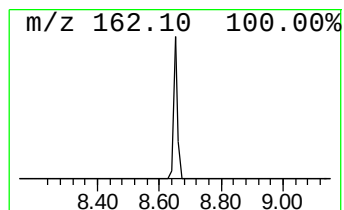
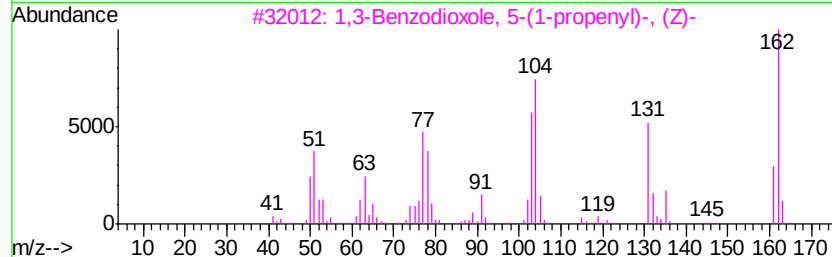
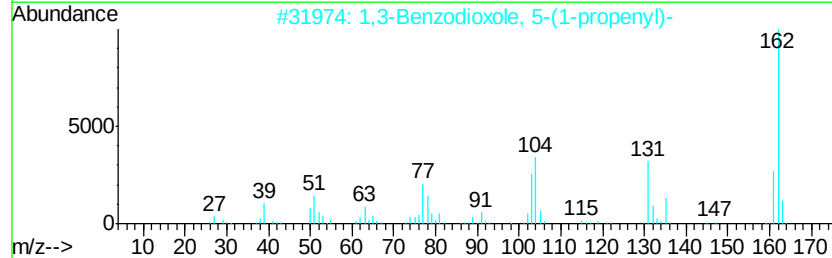
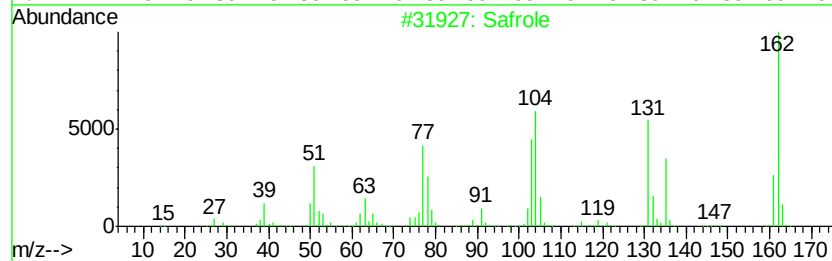
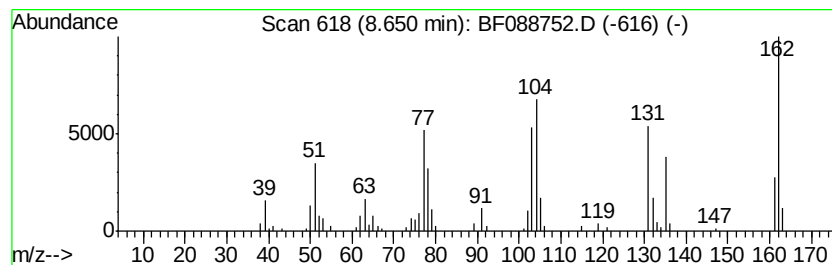
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Peak Number 6 Safrole Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.65	3.79 ng	148389	Napthalene-d8	8.03	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Safrole	162	C10H10O2	000094-59-7	99
2	1,3-Benzodioxole, 5-(1-propenyl)-	162	C10H10O2	000120-58-1	97
3	1,3-Benzodioxole, 5-(1-propenyl)...	162	C10H10O2	017627-76-8	95
4	Benzene, 1,2-(methylenedioxy)-4-...	162	C10H10O2	004043-71-4	95
5	Sydnone, 3-phenyl-	162	C8H6N2O2	000120-06-9	55



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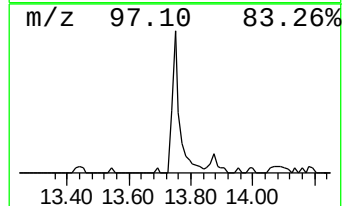
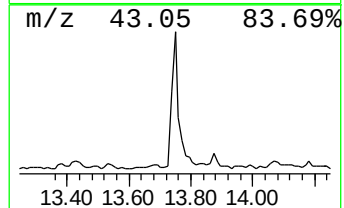
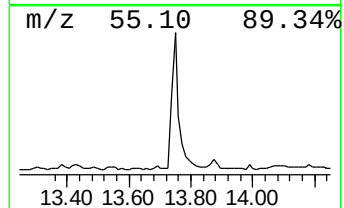
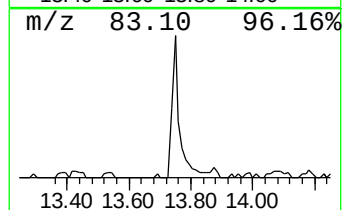
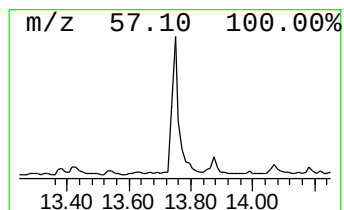
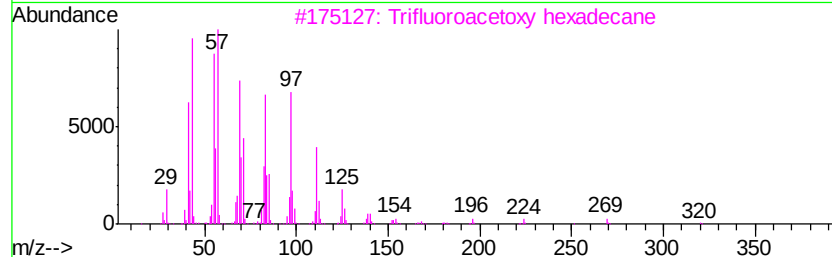
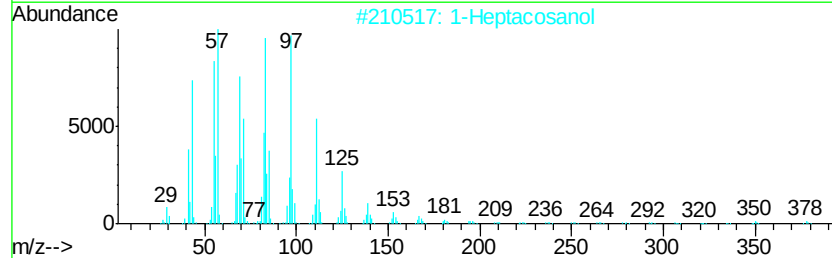
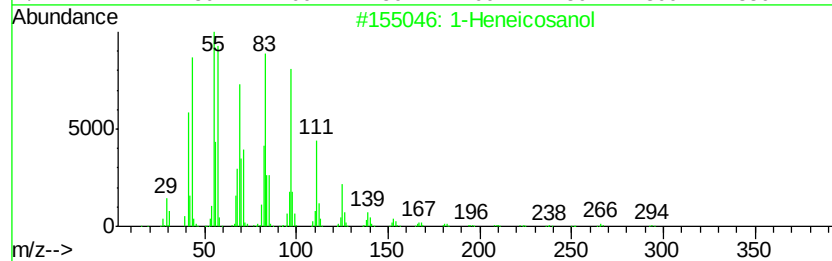
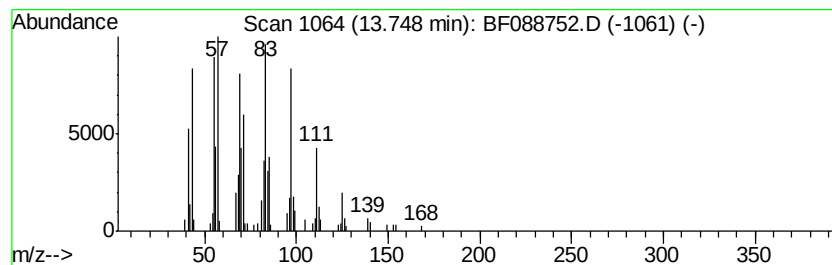
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Peak Number 7 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	5.79 ng	214686	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol		312	C21H44O	015594-90-8	95
2	1-Heptacosanol		396	C27H56O	002004-39-9	94
3	Trifluoroacetoxy hexadecane		338	C18H33F3O2	006222-03-3	94
4	Trichloroacetic acid, hexadecyl ...		386	C18H33Cl3O2	074339-54-1	94
5	n-Nonadecanol-1		284	C19H40O	001454-84-8	91



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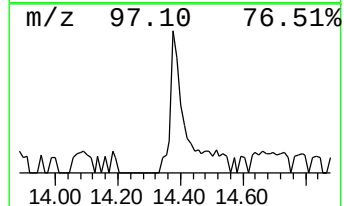
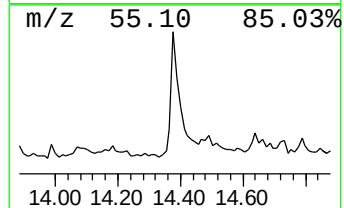
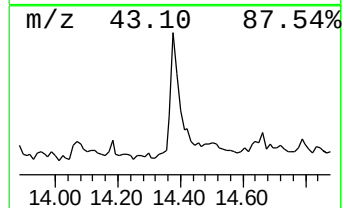
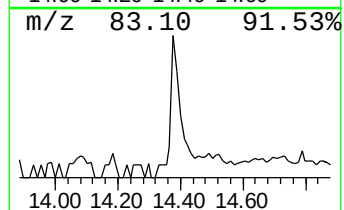
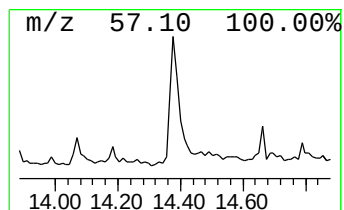
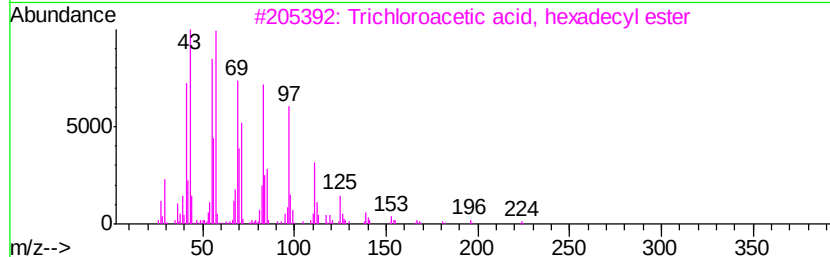
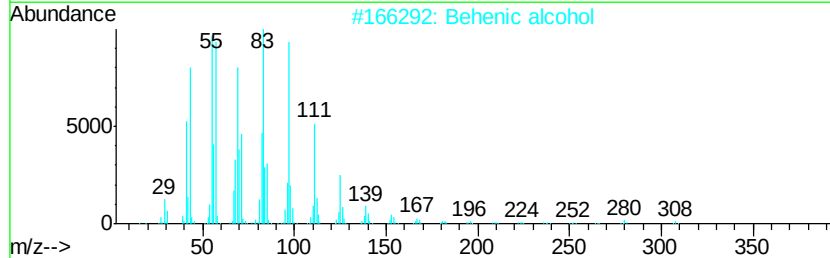
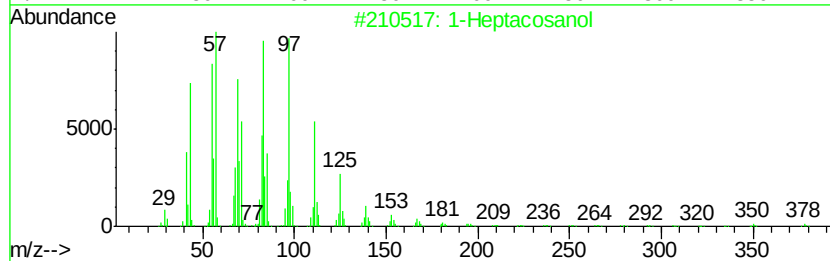
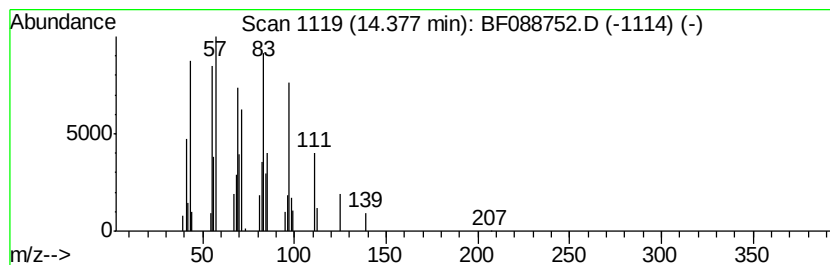
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Peak Number 8 1-Heptacosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.38	2.34 ng	86803	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heptacosanol	396	C27H56O	002004-39-9	94
2		Behenic alcohol	326	C22H46O	000661-19-8	93
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	90



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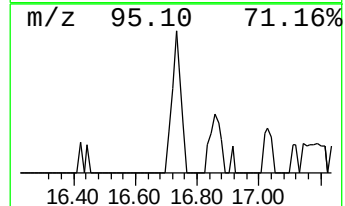
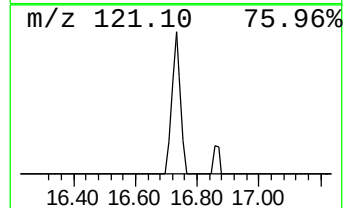
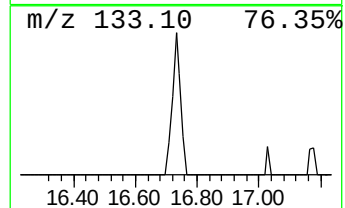
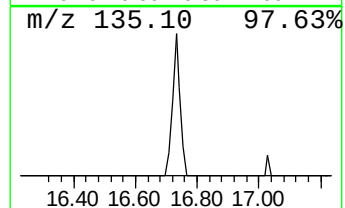
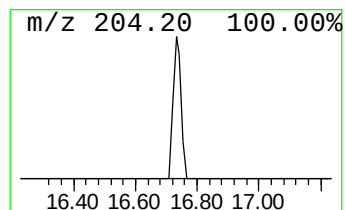
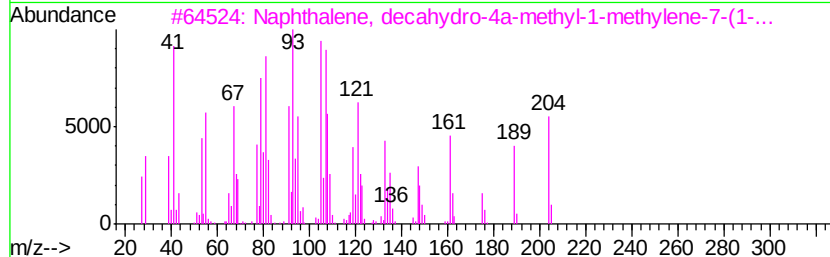
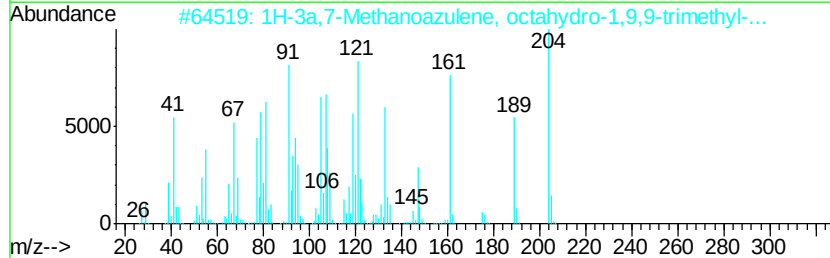
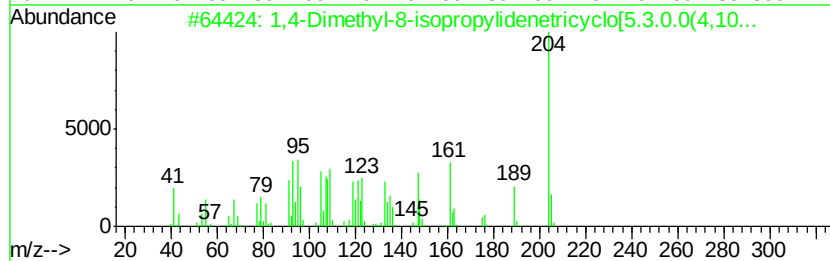
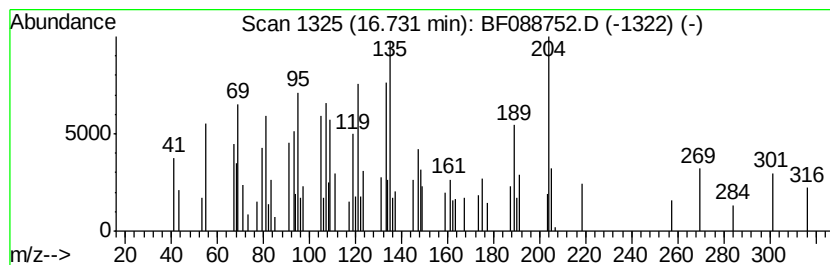
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1,4-Dimethyl-8-isopropylide... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	3.11 ng	81924	Perylene-d12	15.26

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	64
2			1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	53
3			Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	49
4			2H-Cyclopentacyclooctene, 4,5,6,...	204	C15H24	1000221-85-8	45
5			2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H200	124957-09-1	45



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070616\
Data File : BF088752.D
Acq On : 6 Jul 2016 23:56
Operator : UM/SJ
Sample : H3878-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C2.1-09

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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...	4.91	4.5	ng	116375	1	6.74	515049	20.0
unknown6.51	6.51	79.0	ng	2035420	1	6.74	515049	20.0
Safrole	8.65	3.8	ng	148389	2	8.03	782541	20.0
1-Heneicosanol	13.75	5.8	ng	214686	5	13.87	741743	20.0
1-Heptacosanol	14.38	2.3	ng	86803	5	13.87	741743	20.0
1,4-Dimethyl-8-is...	16.73	3.1	ng	81924	6	15.26	527272	20.0