

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100818\
 Data File : BF109664.D
 Acq On : 8 Oct 2018 22:53
 Operator : JU/SJ
 Sample : J5304-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CA-AQIDW-20181004

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-BF100818.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	5.316	546	549	570	rBV	399281	688485	29.10%	4.370%
2	6.345	721	724	741	rBV	226425	550243	23.26%	3.492%
3	6.469	741	745	769	rVB	1394894	1672724	70.70%	10.617%
4	6.698	780	784	806	rVV	407699	596953	25.23%	3.789%
5	6.851	806	810	842	rVB	1473444	1655765	69.98%	10.509%
6	7.263	876	880	914	rBV	926603	1353521	57.21%	8.591%
7	7.975	998	1001	1030	rBV	540142	751087	31.74%	4.767%
8	9.051	1180	1184	1203	rBV	2386849	2366040	100.00%	15.017%
9	9.445	1247	1251	1262	rBV	113844	128234	5.42%	0.814%
10	9.722	1294	1298	1318	rBV2	726637	753377	31.84%	4.782%
11	10.510	1428	1432	1450	rBV	965556	1140739	48.21%	7.240%
12	11.204	1546	1550	1560	rBV	530247	642959	27.17%	4.081%
13	11.739	1637	1641	1645	rBV	19584	24709	1.04%	0.157%
14	12.780	1814	1818	1833	rBV	1830060	1723448	72.84%	10.939%
15	13.686	1966	1972	1984	rBV3	44596	96517	4.08%	0.613%
16	13.827	1992	1996	2008	rVB	535600	582198	24.61%	3.695%
17	14.298	2071	2076	2080	rBV	40415	43332	1.83%	0.275%
18	14.592	2123	2126	2130	rVB	65080	62139	2.63%	0.394%
19	14.662	2134	2138	2142	rBV	72881	72592	3.07%	0.461%
20	14.904	2175	2179	2183	rBV	81233	83859	3.54%	0.532%
21	15.221	2228	2233	2236	rBV	373441	462935	19.57%	2.938%
22	15.251	2236	2238	2246	rVB	101395	122795	5.19%	0.779%
23	15.645	2300	2305	2313	rVB	64894	90783	3.84%	0.576%
24	16.103	2378	2383	2391	rVB4	38250	63520	2.68%	0.403%
25	16.639	2469	2474	2481	rBV5	13634	26433	1.12%	0.168%

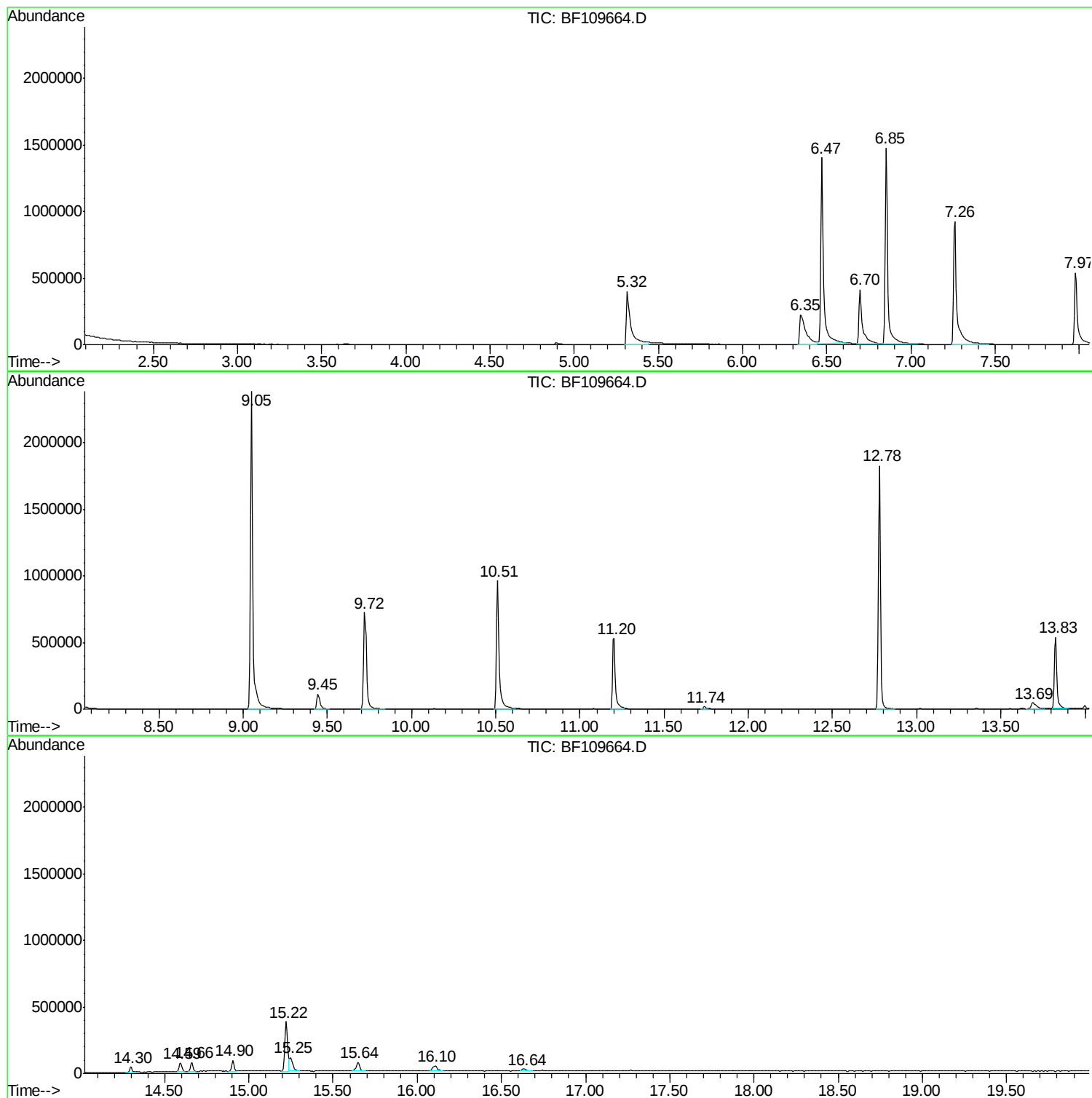
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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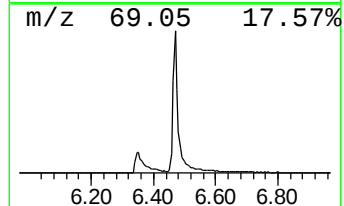
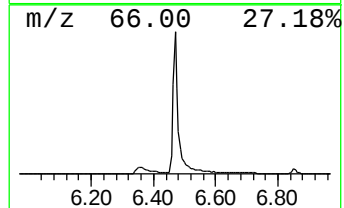
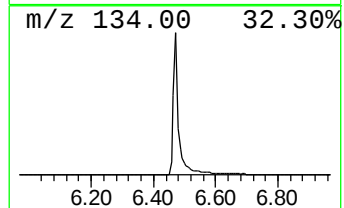
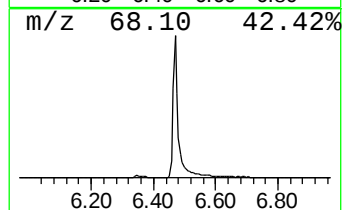
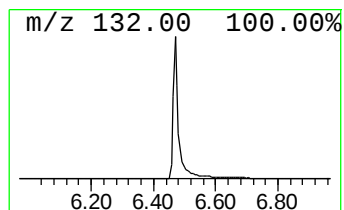
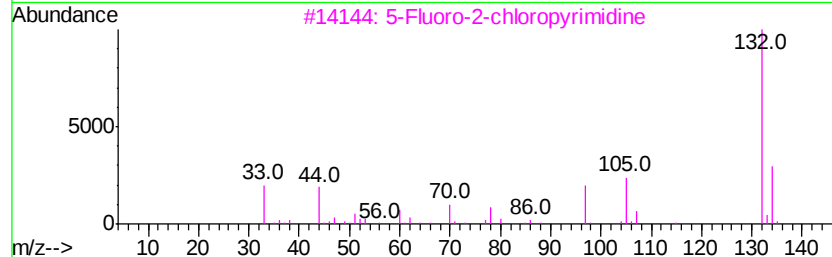
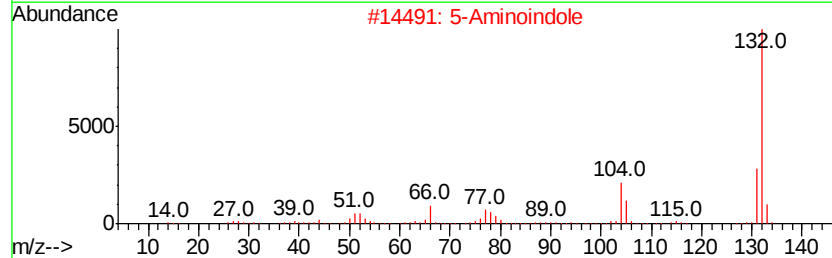
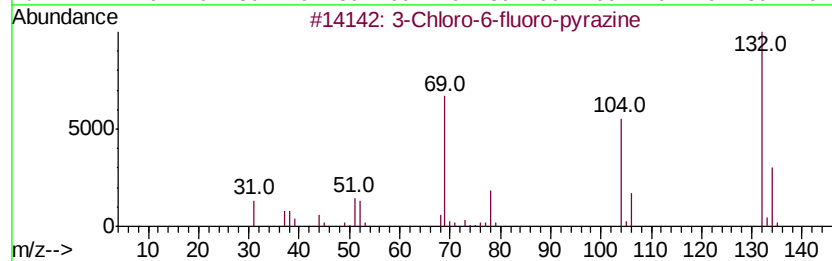
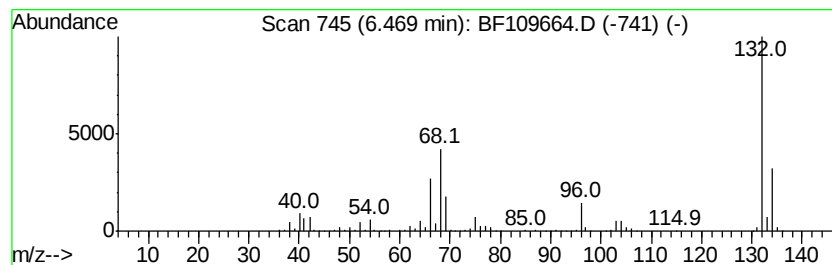
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	56.04 ng	1672720	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5			1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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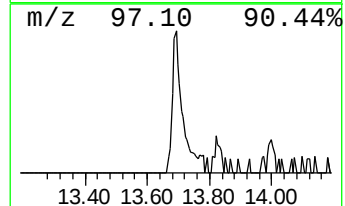
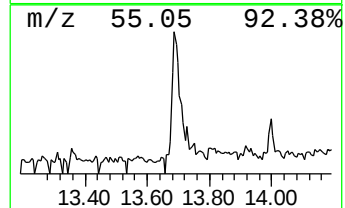
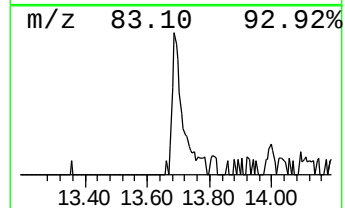
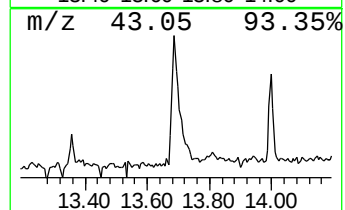
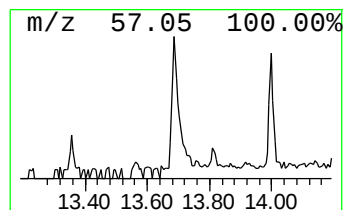
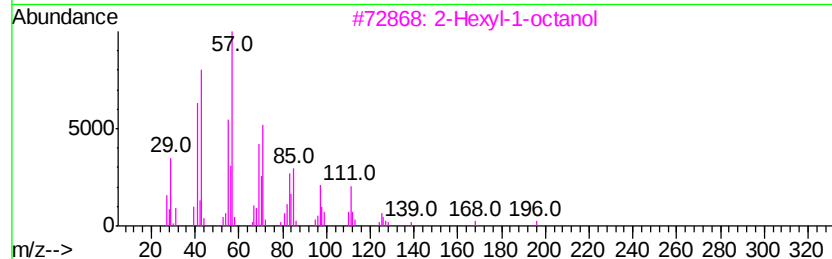
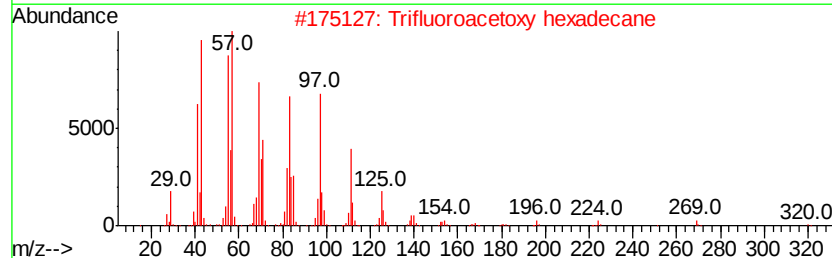
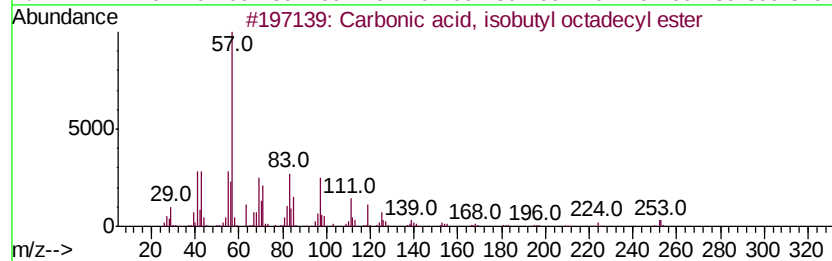
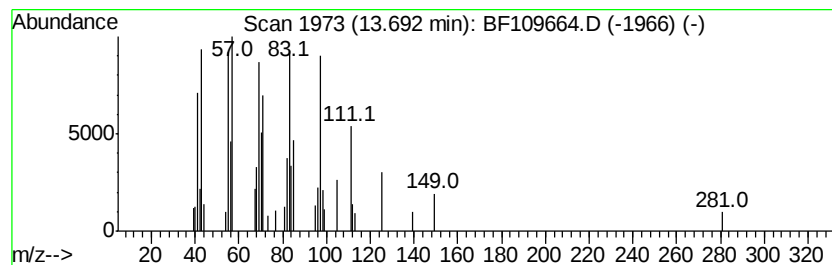
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Peak Number 3 Carbonic acid, isobutyl oct... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	3.32 ng	96517	Chrysene-d12	13.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Carbonic acid, isobutyl octadecyl...	370	C23H46O3	1000314-61-5	80
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	74
3		2-Hexyl-1-octanol	214	C14H30O	019780-79-1	72
4		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	72
5		1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	72



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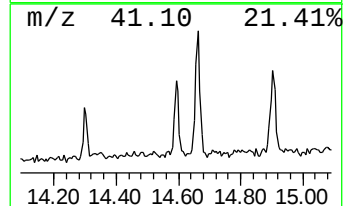
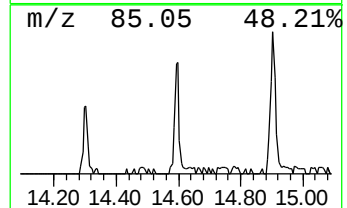
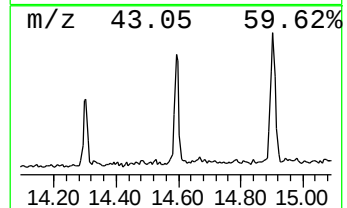
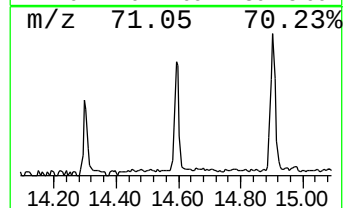
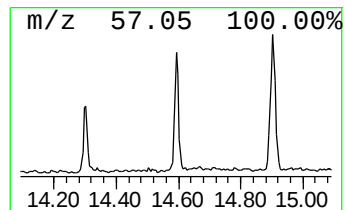
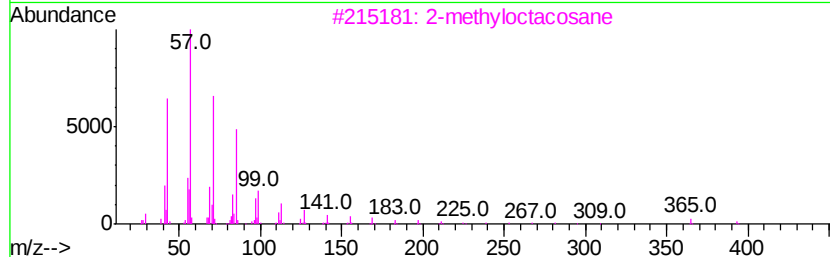
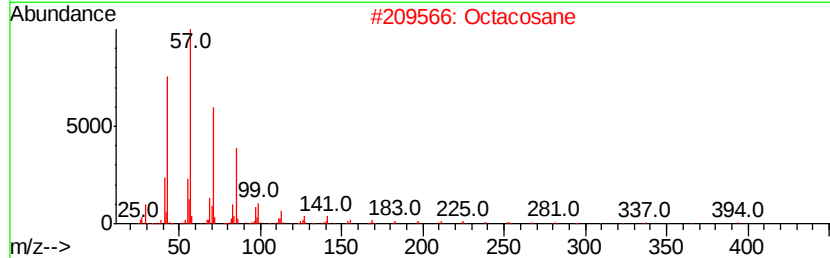
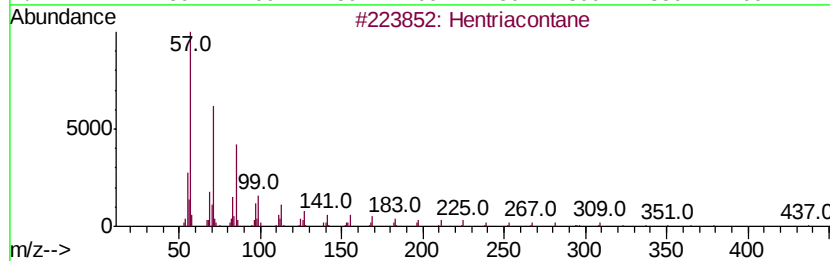
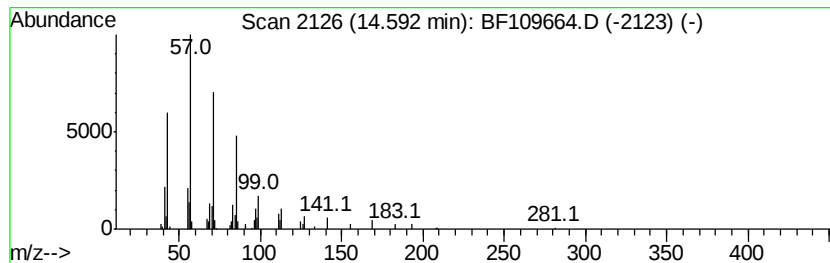
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Peak Number 4 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	2.68 ng	62139	Perylene-d12	15.22

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	2-methyloctacosane		408	C29H60	1000376-72-8	91
4	Octadecane		254	C18H38	000593-45-3	91
5	Hexacosane		366	C26H54	000630-01-3	90



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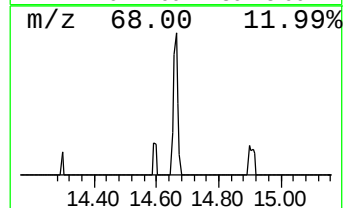
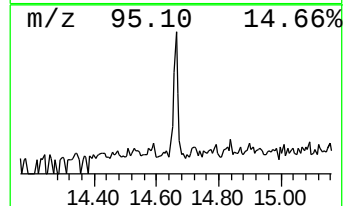
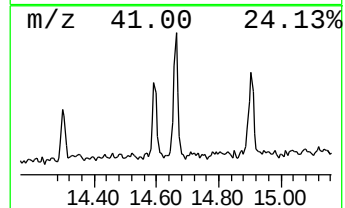
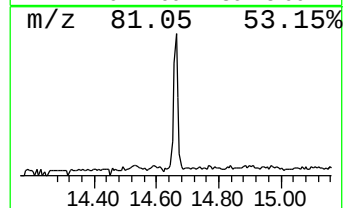
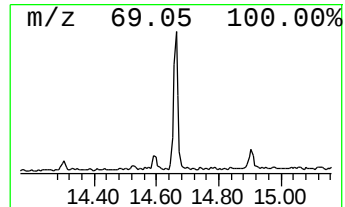
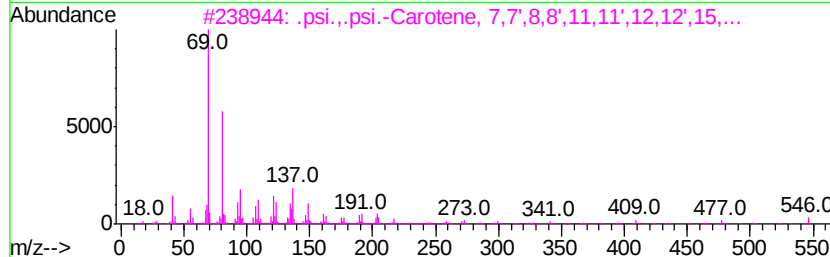
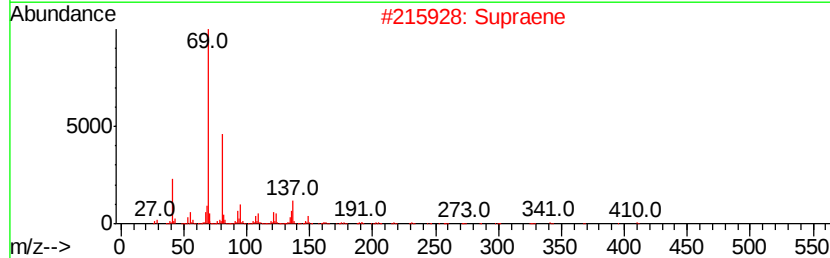
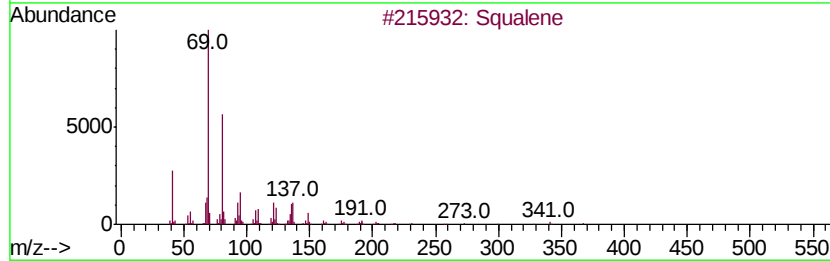
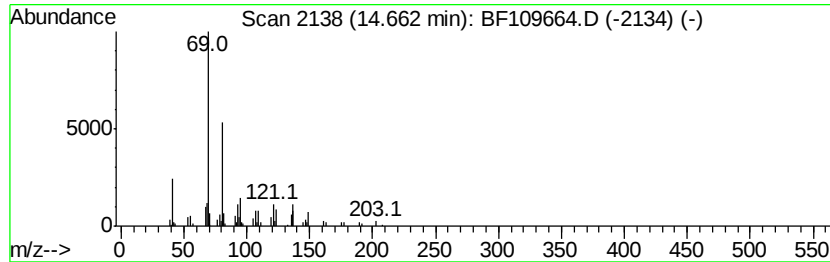
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Peak Number 5 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	3.14 ng	72592	Perylene-d12	15.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		.psi.,.psi.-Carotene, 7,7',8,8',....	547	C40H66	000502-62-5	83
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5		trans-Farnesol	222	C15H26O	000106-28-5	72



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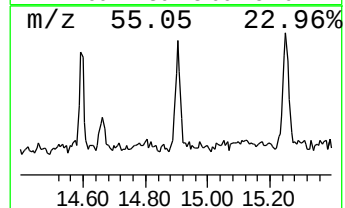
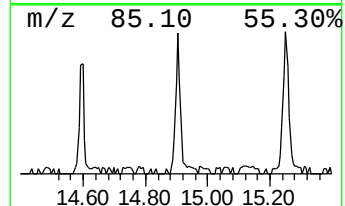
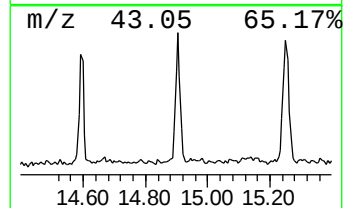
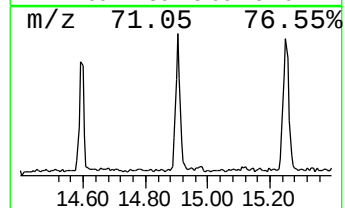
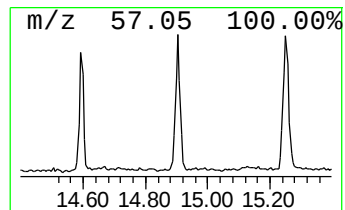
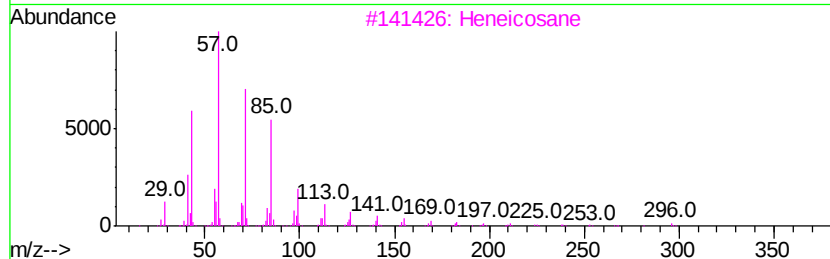
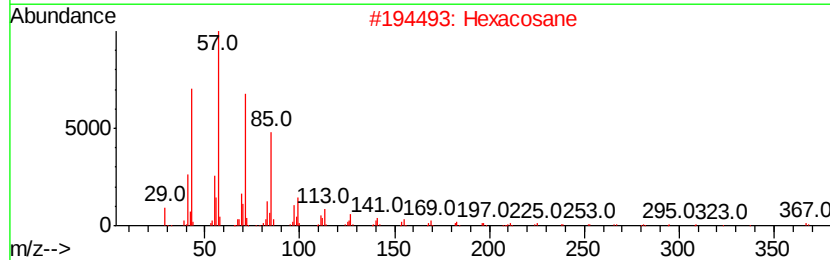
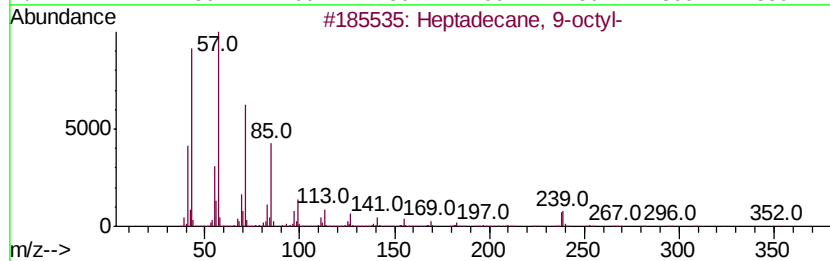
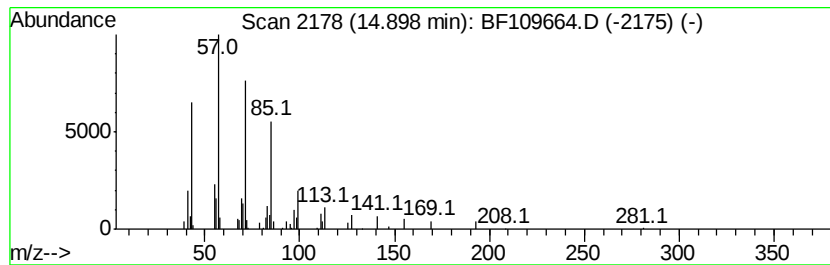
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.90	3.62 ng	83859	Perylene-d12	15.22	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91



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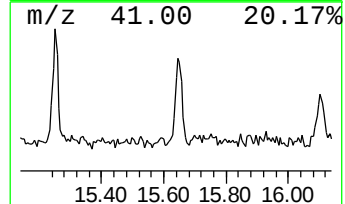
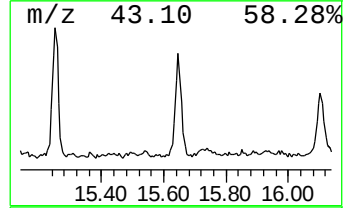
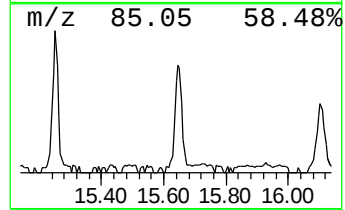
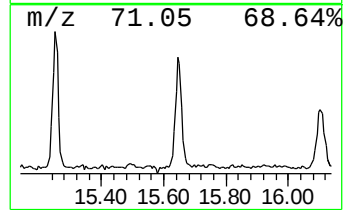
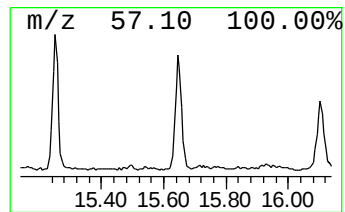
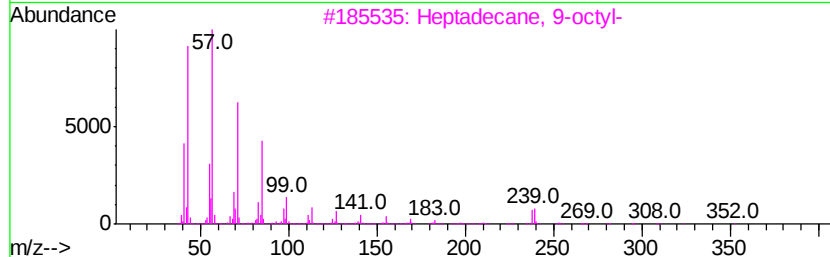
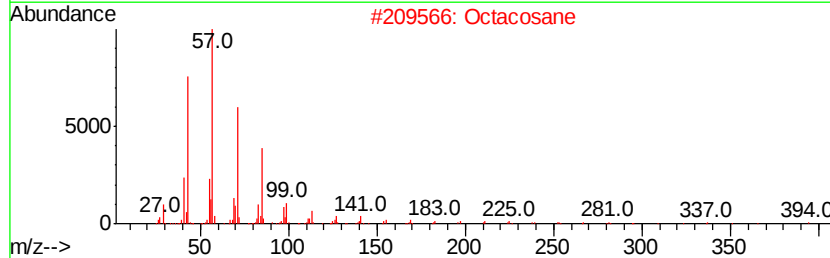
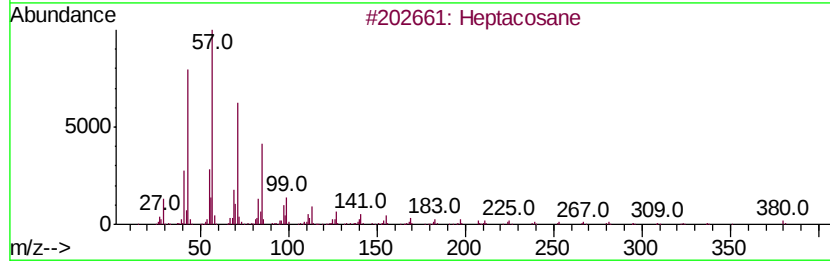
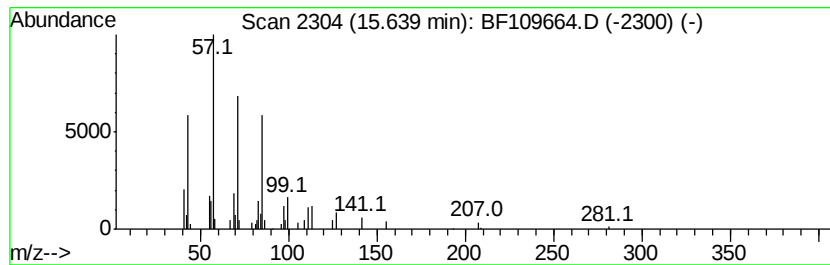
Instrument :
BNA_F
ClientSampleId :
CA-AQIDW-20181004

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	3.92 ng	90783	Perylene-d12	15.22
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptacosane	380 C27H56	000593-49-7	91
2	Octacosane	394 C28H58	000630-02-4	91
3	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	91
4	Heneicosane	296 C21H44	000629-94-7	91
5	Hentriacontane	437 C31H64	000630-04-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109664.D
Acq On : 8 Oct 2018 22:53
Operator : JU/SJ
Sample : J5304-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CA-AQIDW-20181004

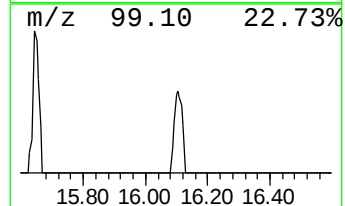
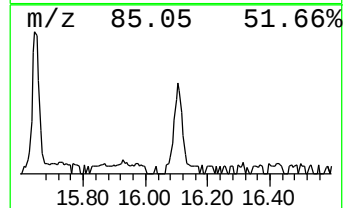
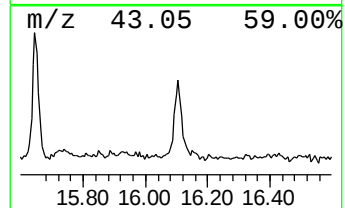
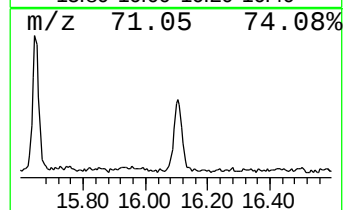
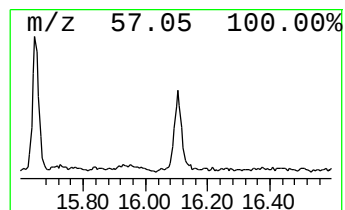
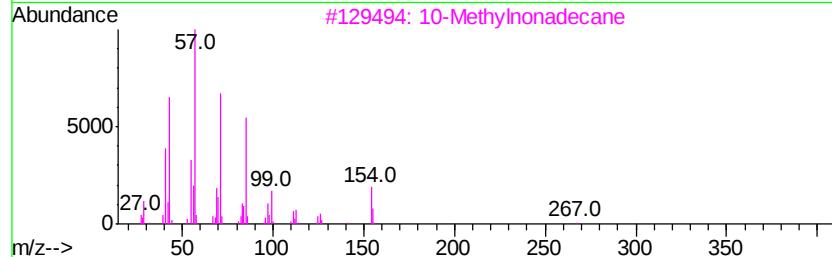
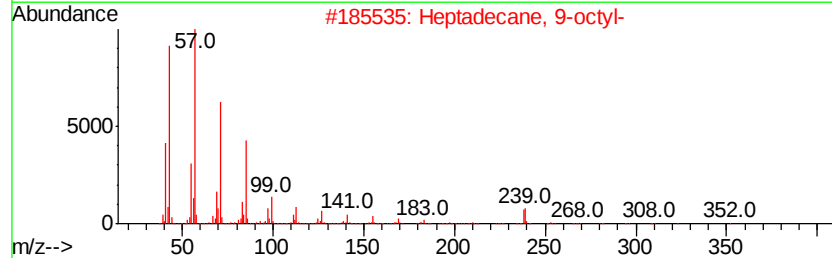
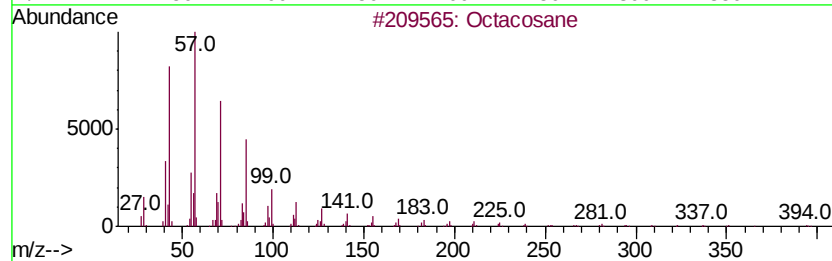
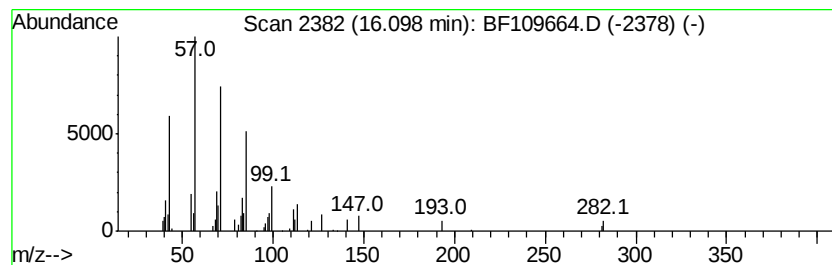
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	2.74 ng	63520	Perylene-d12	15.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3		10-Methylnonadecane	282	C20H42	056862-62-5	87
4		Heneicosane	296	C21H44	000629-94-7	87
5		Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100818\
Data File : BF109664.D
Acq On : 8 Oct 2018 22:53
Operator : JU/SJ
Sample : J5304-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CA-AQIDW-20181004

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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
unknown6.47	6.47	56.0	ng	1672720	1	6.70	596953	20.0
Carbonic acid, is...	13.69	3.3	ng	96517	5	13.83	582198	20.0
Hentriacontane	14.59	2.7	ng	62139	6	15.22	462935	20.0
Squalene	14.66	3.1	ng	72592	6	15.22	462935	20.0
Heptadecane, 9-oc...	14.90	3.6	ng	83859	6	15.22	462935	20.0
Heptacosane	15.64	3.9	ng	90783	6	15.22	462935	20.0
Octacosane	16.10	2.7	ng	63520	6	15.22	462935	20.0