

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112717\
 Data File : BF100882.D
 Acq On : 27 Nov 2017 10:51
 Operator : SJ/JU
 Sample : PB104481BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB104481BL

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-BF110817.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	5.087	505	510	521	rBB	80633	105734	5.20%	0.655%
2	5.481	572	577	580	rBV	1476956	1419393	69.75%	8.794%
3	6.492	743	749	751	rBV	1323836	1463701	71.93%	9.068%
4	6.628	767	772	775	rBV	1669924	1525105	74.95%	9.449%
5	6.857	807	811	814	rBV	491891	387593	19.05%	2.401%
6	7.016	833	838	841	rBV	1371726	1215291	59.72%	7.529%
7	7.422	901	907	910	rBV	1004132	954968	46.93%	5.916%
8	7.492	915	919	923	rBV	40142	31041	1.53%	0.192%
9	8.139	1021	1029	1032	rBV	634169	532871	26.19%	3.301%
10	9.216	1206	1212	1215	rBV	2207196	2004416	98.50%	12.418%
11	9.245	1215	1217	1221	rVB	70117	53672	2.64%	0.333%
12	9.286	1221	1224	1227	rBV	32242	25762	1.27%	0.160%
13	9.351	1232	1235	1241	rVB	43423	40018	1.97%	0.248%
14	9.604	1274	1278	1281	rBV	159957	130578	6.42%	0.809%
15	9.816	1308	1314	1318	rVB	72575	67028	3.29%	0.415%
16	9.892	1323	1327	1331	rBV	672977	622106	30.57%	3.854%
17	10.286	1385	1394	1396	rBV2	40335	47430	2.33%	0.294%
18	10.316	1396	1399	1402	rVB	72963	56307	2.77%	0.349%
19	10.533	1430	1436	1439	rBV3	14987	22359	1.10%	0.139%
20	10.686	1457	1462	1465	rBV	1285833	1197269	58.84%	7.418%
21	10.786	1477	1479	1484	rVB	45895	41520	2.04%	0.257%
22	11.380	1576	1580	1583	rBV	825816	674470	33.14%	4.179%
23	11.898	1663	1668	1672	rBV	56190	58546	2.88%	0.363%
24	12.680	1793	1801	1808	rBV2	42924	63157	3.10%	0.391%
25	12.968	1845	1850	1853	rBV	2118809	2034916	100.00%	12.607%
26	13.851	1996	2000	2003	rBV	129636	133883	6.58%	0.829%
27	13.886	2003	2006	2011	rVB	185289	168231	8.27%	1.042%
28	14.021	2025	2029	2032	rBV	651910	562787	27.66%	3.487%
29	15.127	2209	2217	2218	rBV2	29026	49210	2.42%	0.305%
30	15.492	2273	2279	2286	rBV	314247	410787	20.19%	2.545%
31	16.968	2522	2530	2536	rBV9	14148	40856	2.01%	0.253%

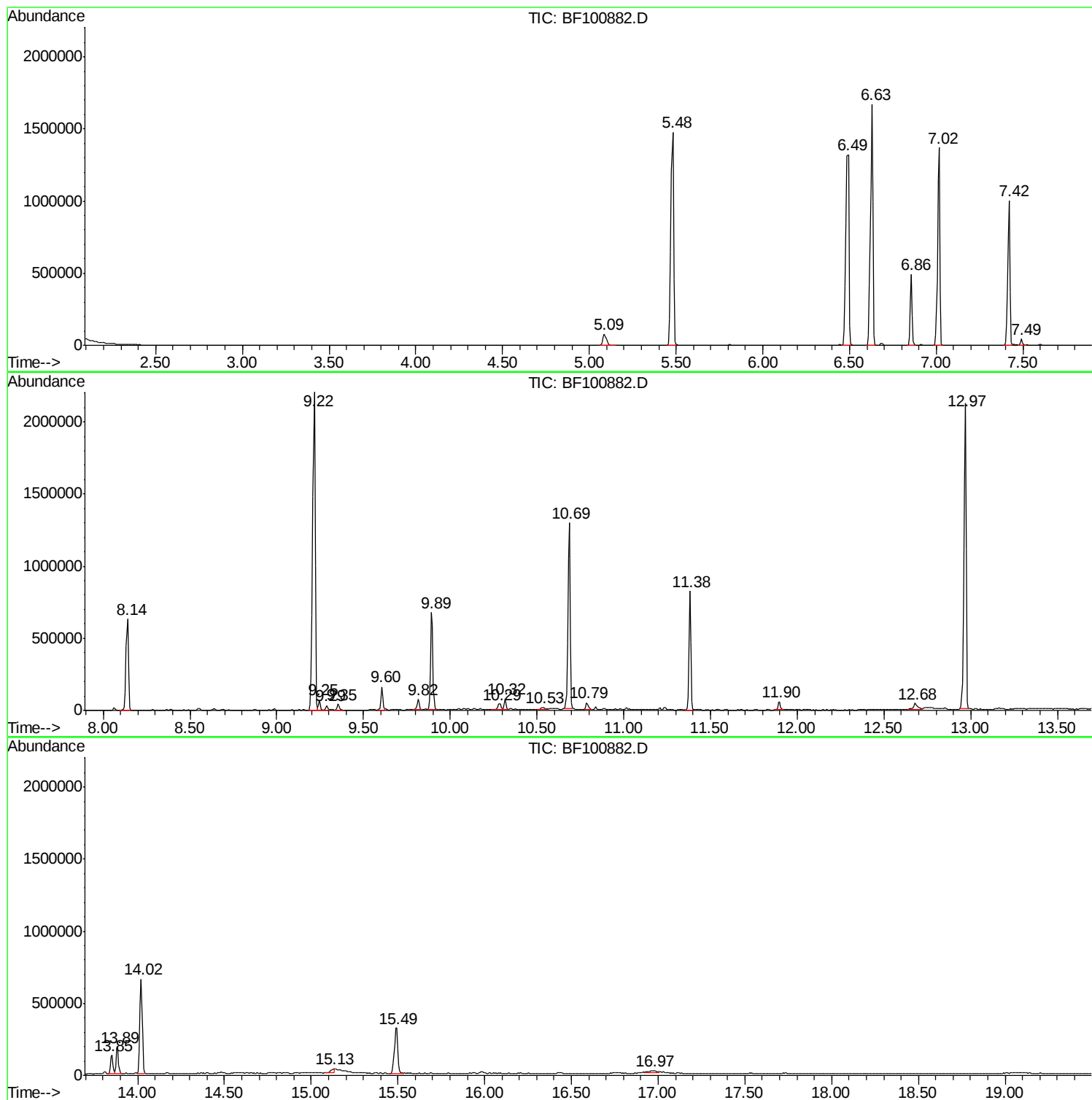
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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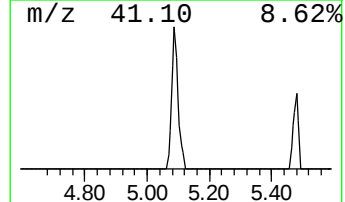
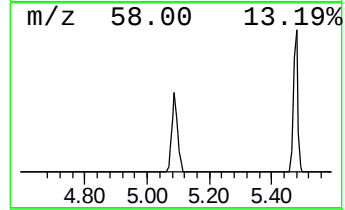
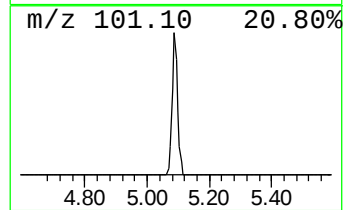
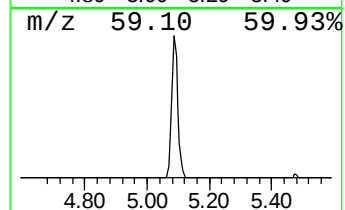
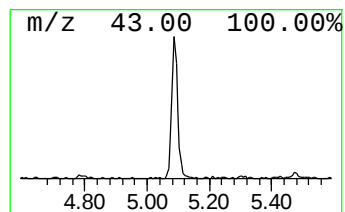
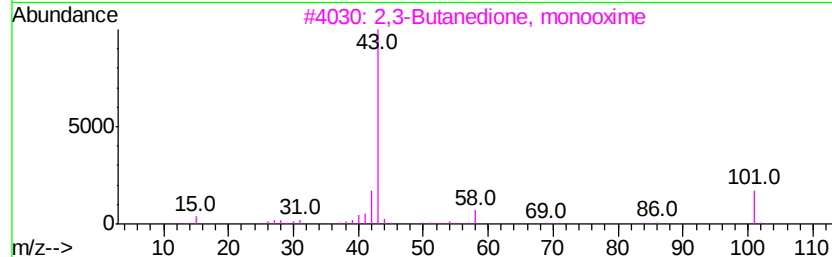
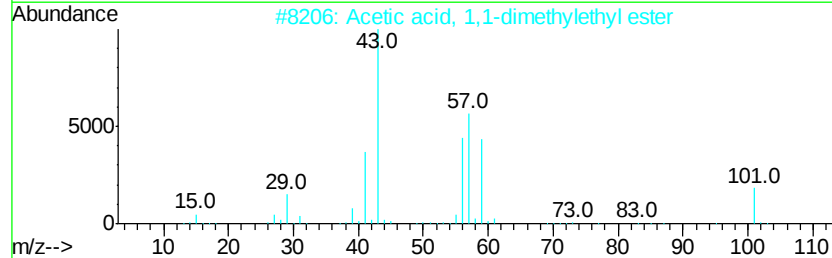
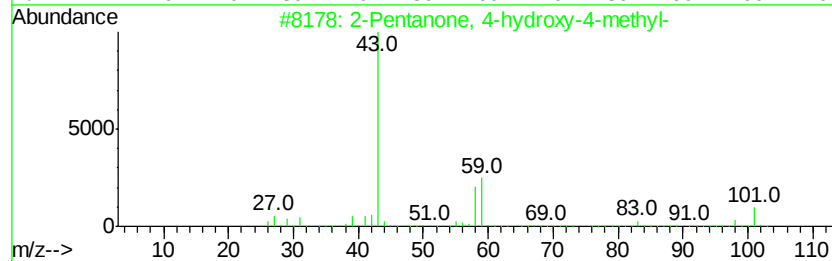
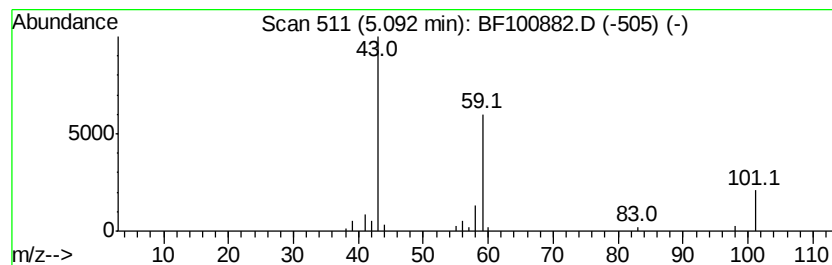
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	5.46 ng	105734	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4			3-Hexanol	102	C6H14O	000623-37-0	33
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25



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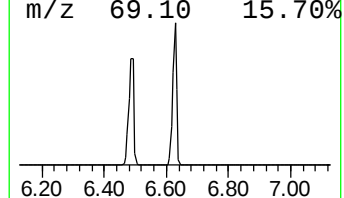
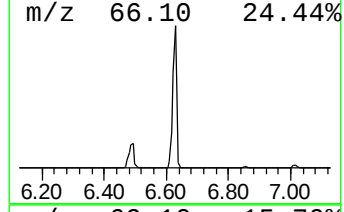
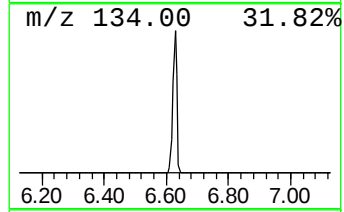
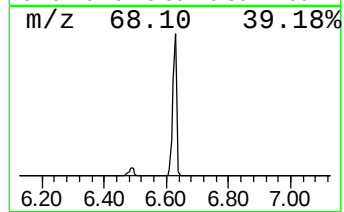
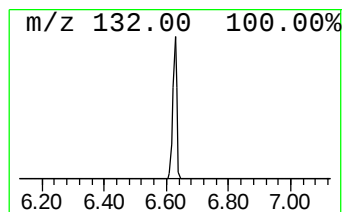
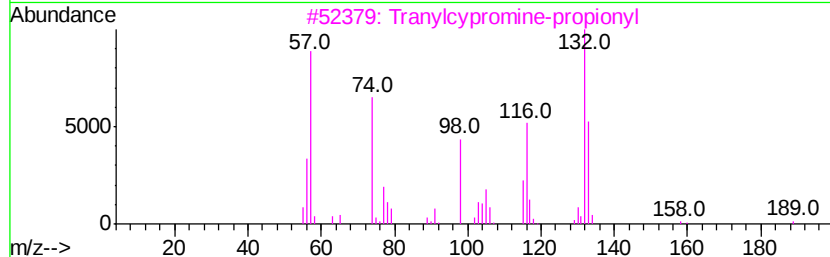
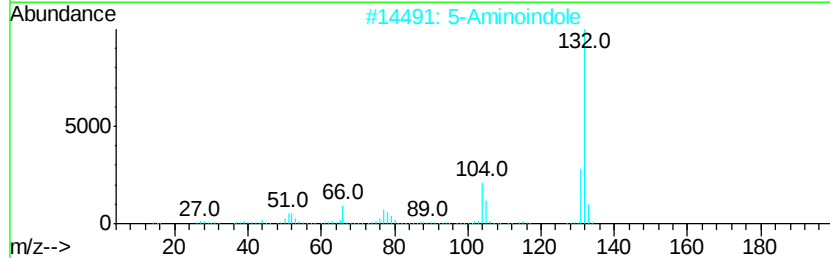
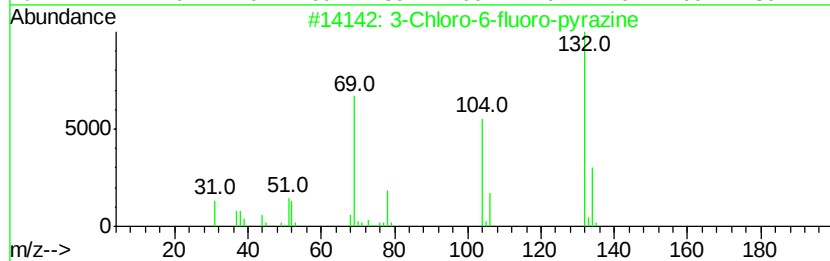
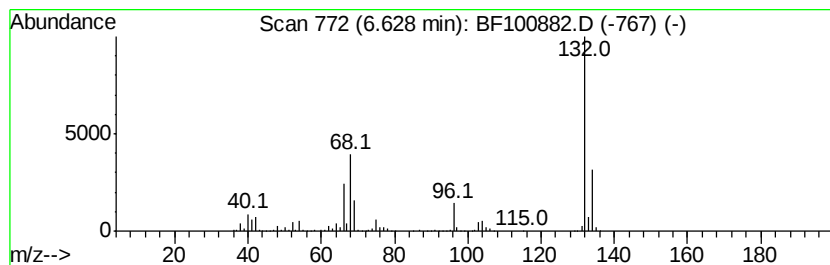
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Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	78.70 ng	1525110	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16	
2	5-Aminoindole	132	C8H8N2	005192-03-0	12	
3	Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10	
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9	
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9	



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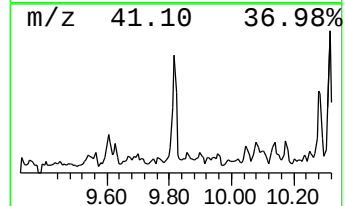
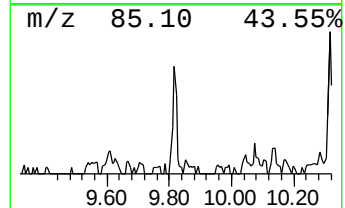
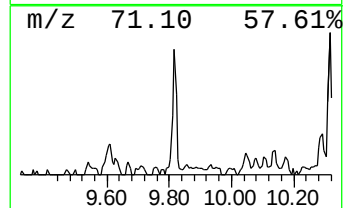
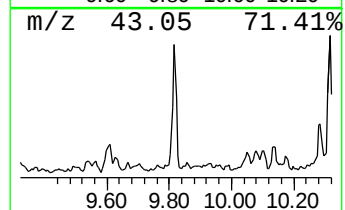
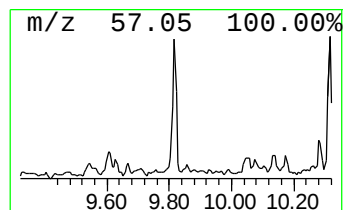
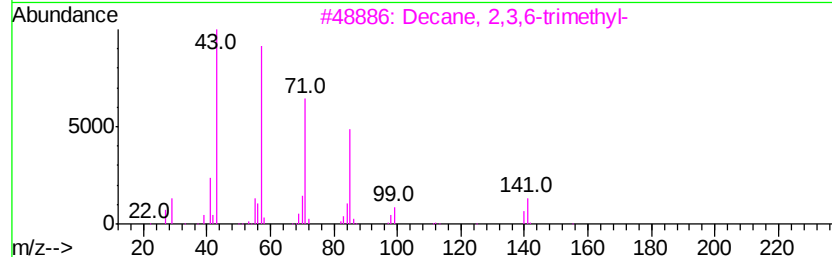
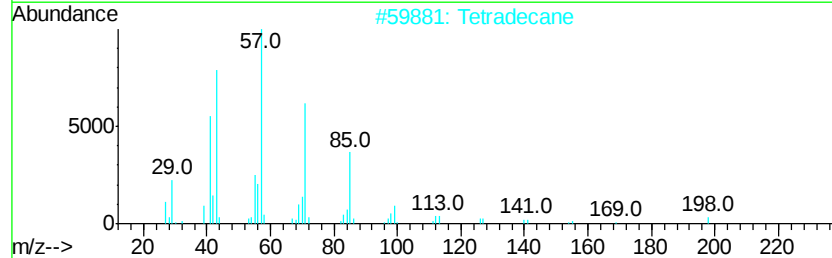
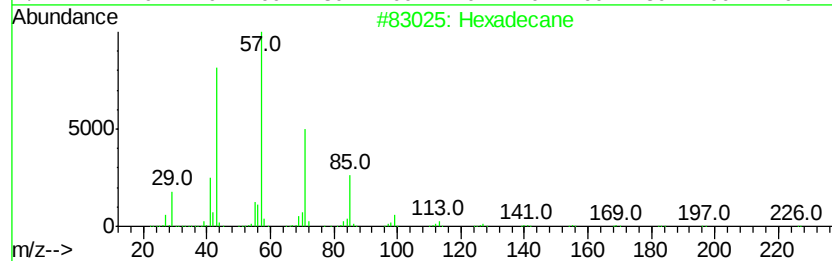
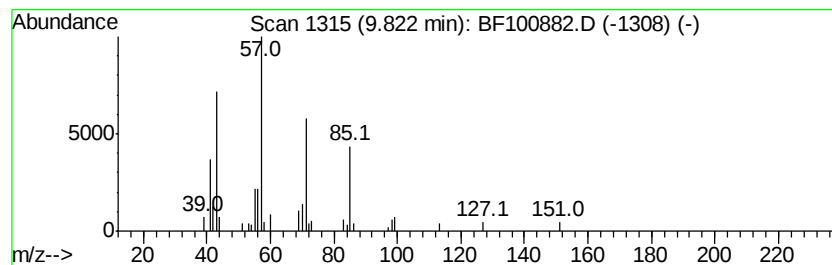
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Peak Number 4 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.82	2.15 ng	67028	Acenaphthene-d10	9.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	86
2		Tetradecane	198	C14H30	000629-59-4	72
3		Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	64
4		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	64
5		Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	64



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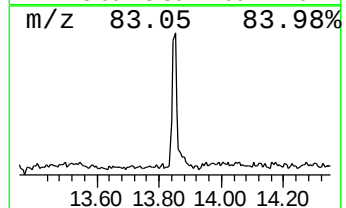
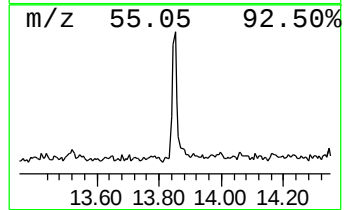
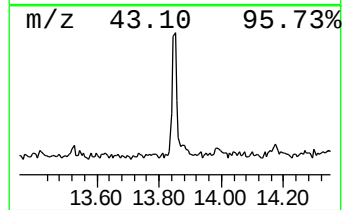
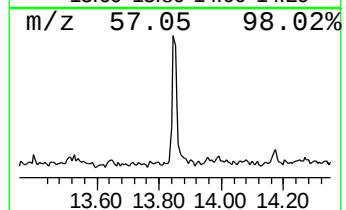
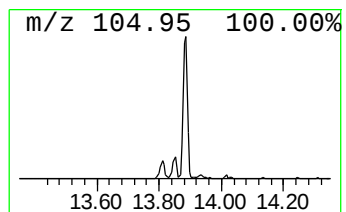
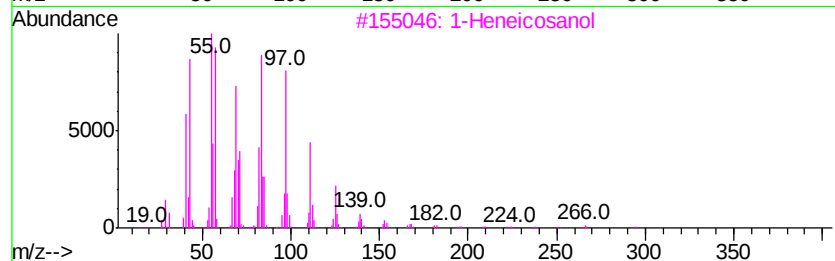
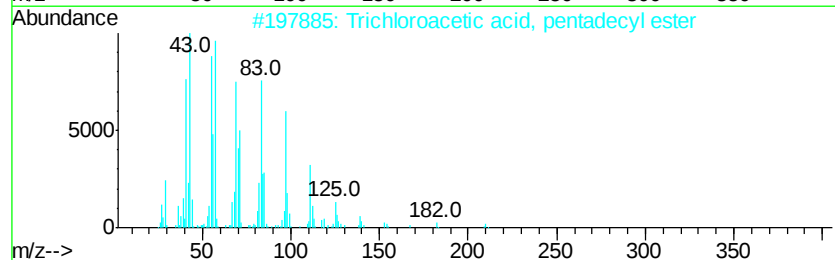
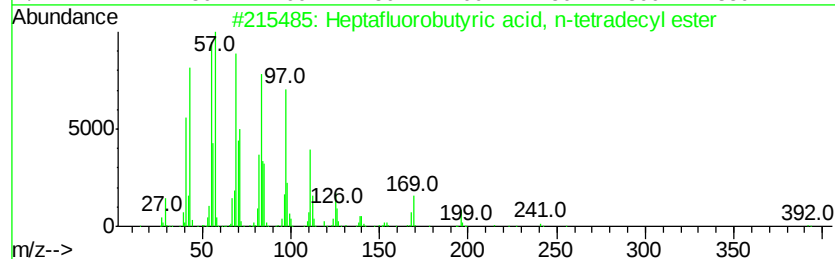
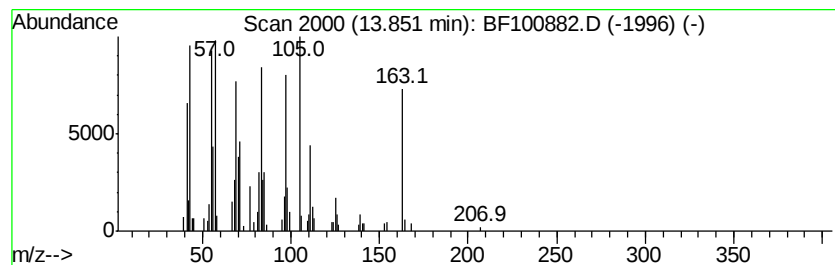
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Peak Number 5 Heptafluorobutyric acid, n-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	4.76 ng	133883	Chrysene-d12	14.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	90
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
3		1-Heneicosanol	312	C21H44O	015594-90-8	90
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	87
5		Behenic alcohol	326	C22H46O	000661-19-8	81



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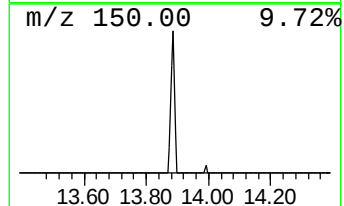
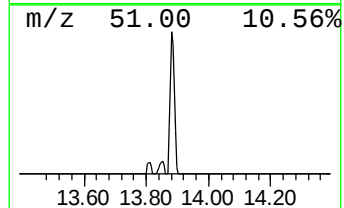
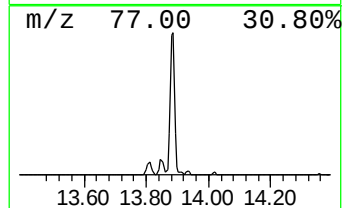
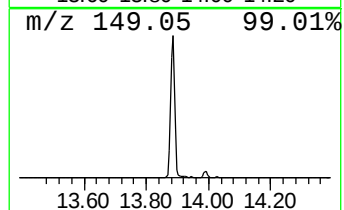
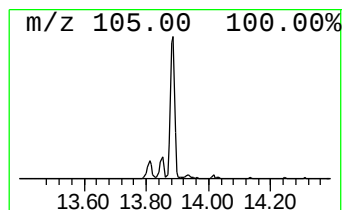
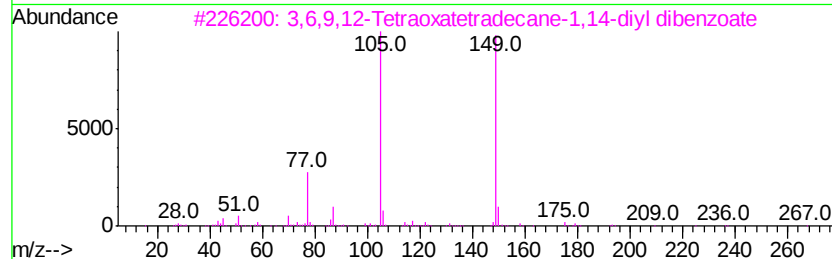
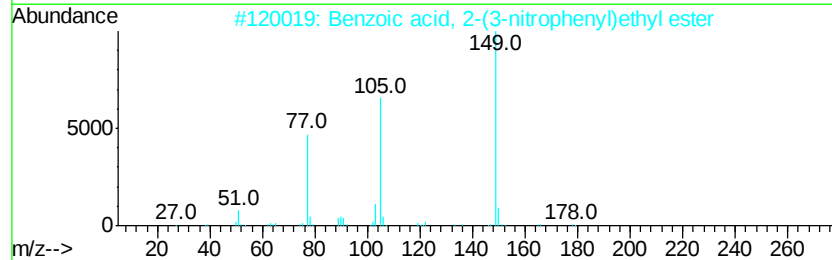
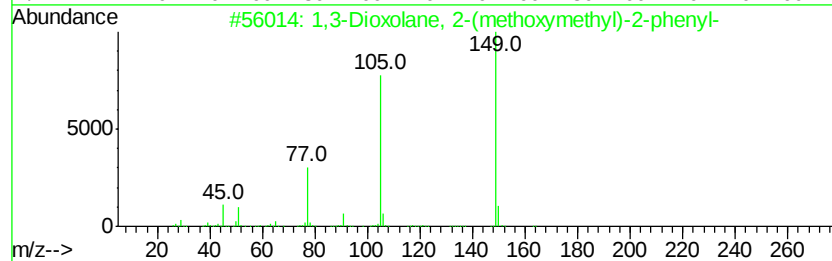
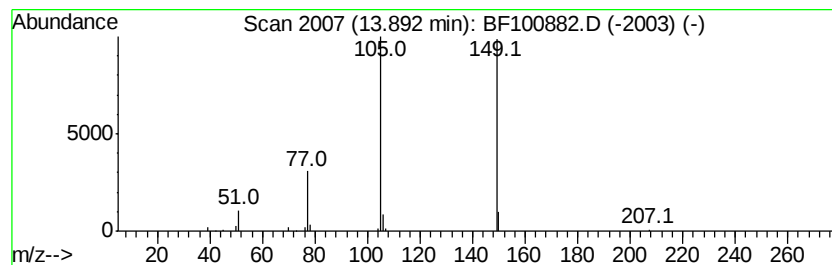
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Peak Number 6 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	5.98 ng	168231	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	83
2		Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	78
3		3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	64
4		2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	58
5		Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	56



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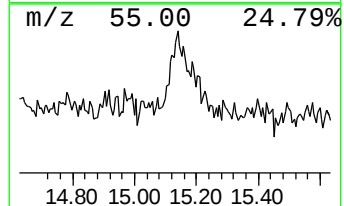
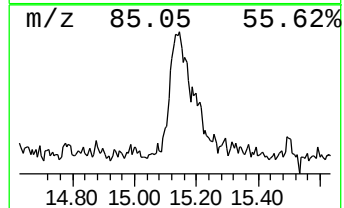
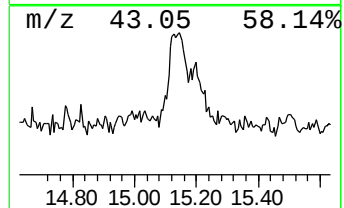
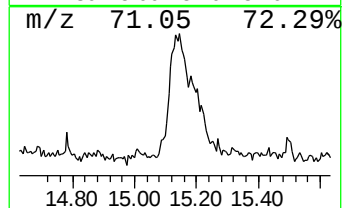
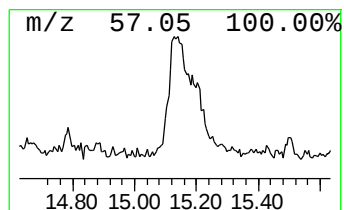
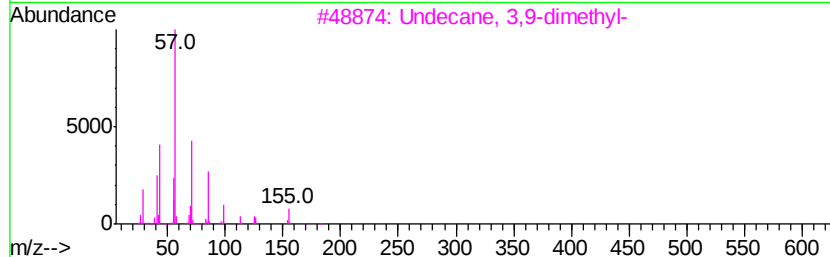
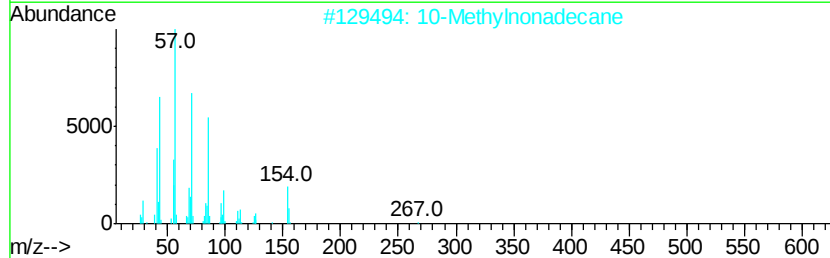
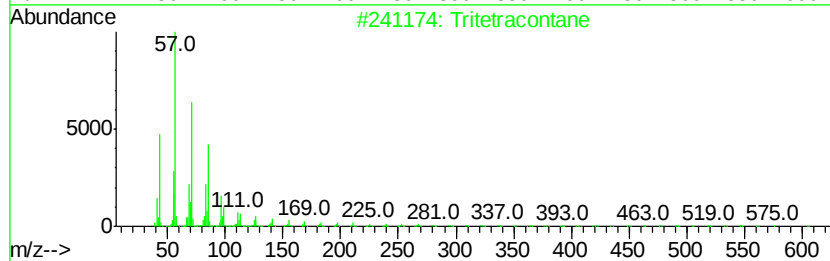
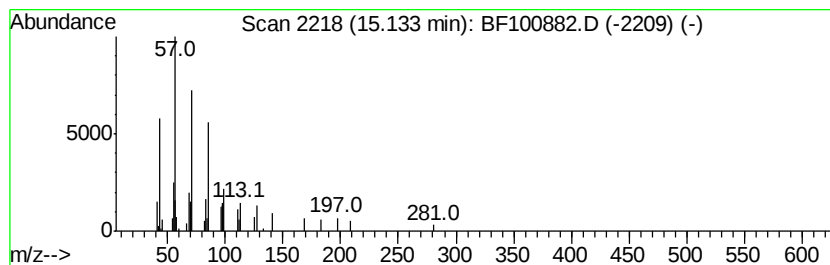
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tritetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	2.40 ng	49210	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tritetracontane	605	C43H88	007098-21-7	72
2		10-Methylnonadecane	282	C20H42	056862-62-5	64
3		Undecane, 3,9-dimethyl-	184	C13H28	017301-31-4	64
4		Octacosane	394	C28H58	000630-02-4	59
5		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112717\
Data File : BF100882.D
Acq On : 27 Nov 2017 10:51
Operator : SJ/JU
Sample : PB104481BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB104481BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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...	5.09	5.5	ng	105734	1	6.86	387593	20.0
unknown6.63	6.63	78.7	ng	1525110	1	6.86	387593	20.0
Hexadecane	9.82	2.1	ng	67028	3	9.89	622106	20.0
Heptafluorobutyri...	13.85	4.8	ng	133883	5	14.02	562787	20.0
1,3-Dioxolane, 2-...	13.89	6.0	ng	168231	5	14.02	562787	20.0
Tritetracontane	15.13	2.4	ng	49210	6	15.49	410787	20.0