

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100317\
 Data File : BF099039.D
 Acq On : 3 Oct 2017 19:25
 Operator : SJ/JU
 Sample : I5496-03
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PAMT-COMP-B

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-BF092317.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	2.157	7	12	26	rVB	482878	632186	26.39%	3.621%
2	2.281	30	33	39	rVB	26050	34361	1.43%	0.197%
3	2.993	149	154	162	rVB	27180	41826	1.75%	0.240%
4	4.440	396	400	406	rBV	60622	67876	2.83%	0.389%
5	4.887	472	476	481	rBV	36237	36377	1.52%	0.208%
6	5.081	506	509	518	rVB	256686	261130	10.90%	1.496%
7	5.481	574	577	581	rBV	672565	594807	24.83%	3.407%
8	6.487	745	748	755	rVB2	479631	494080	20.62%	2.830%
9	6.634	769	773	777	rBV	1119536	1012386	42.26%	5.798%
10	6.869	810	813	817	rBV	847610	725765	30.30%	4.157%
11	7.028	829	840	843	rBV	1885464	1610227	67.22%	9.222%
12	7.434	904	909	912	rBV	1441550	1283626	53.58%	7.351%
13	8.151	1027	1031	1035	rBV	1129605	989842	41.32%	5.669%
14	9.228	1209	1214	1217	rBV	2723840	2395559	100.00%	13.720%
15	9.616	1277	1280	1284	rBV	332127	269581	11.25%	1.544%
16	9.910	1325	1330	1333	rVB	1193025	1083921	45.25%	6.208%
17	10.327	1395	1401	1404	rBV2	59007	69458	2.90%	0.398%
18	10.416	1413	1416	1419	rBV	61823	55434	2.31%	0.317%
19	10.551	1435	1439	1441	rBV	31369	35445	1.48%	0.203%
20	10.692	1460	1463	1469	rVB	808547	664129	27.72%	3.804%
21	10.804	1479	1482	1491	rBV	92248	130263	5.44%	0.746%
22	11.251	1555	1558	1560	rBV	59204	46666	1.95%	0.267%
23	11.280	1560	1563	1566	rVB2	34618	32276	1.35%	0.185%
24	11.392	1578	1582	1586	rBV	1230297	1070325	44.68%	6.130%
25	11.598	1614	1617	1620	rBV3	22684	26027	1.09%	0.149%
26	12.863	1830	1832	1836	rBV	74980	66249	2.77%	0.379%
27	12.980	1847	1852	1855	rVB	2089382	1945369	81.21%	11.141%
28	13.521	1942	1944	1949	rBV2	25285	32551	1.36%	0.186%
29	13.863	1999	2002	2009	rVB2	53807	63912	2.67%	0.366%
30	14.004	2022	2026	2028	rBV	158415	141115	5.89%	0.808%
31	14.033	2028	2031	2034	rVB	802473	697393	29.11%	3.994%
32	14.868	2170	2173	2177	rBV	98842	106935	4.46%	0.612%
33	15.504	2276	2281	2290	rBV2	459065	567810	23.70%	3.252%
34	15.951	2353	2357	2362	rVB3	17329	27070	1.13%	0.155%

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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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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35	16.456	2438	2443	2456	rVB8	28156	66392	2.77%	0.380%
36	17.562	2626	2631	2642	rBV6	30768	82544	3.45%	0.473%

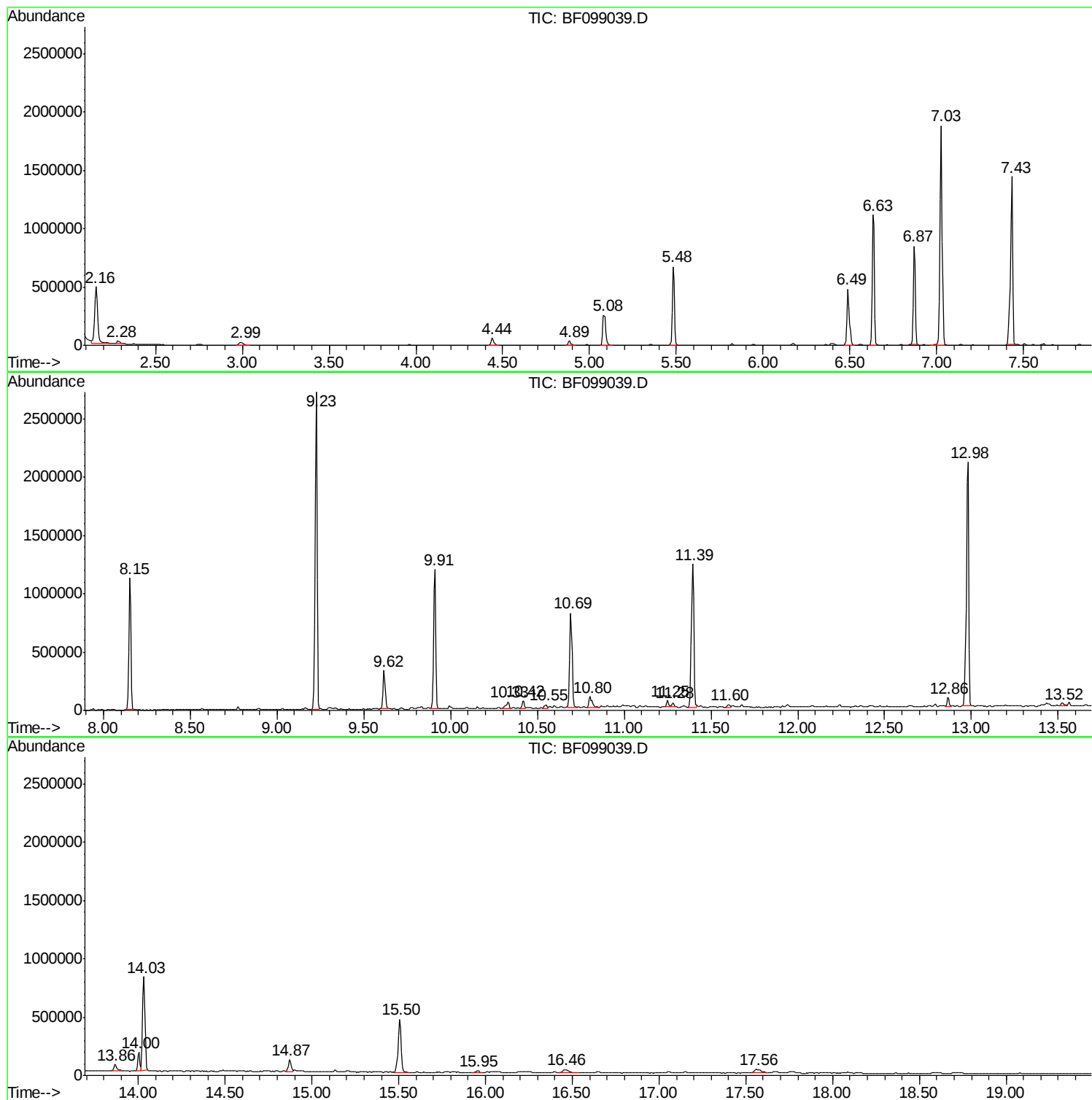
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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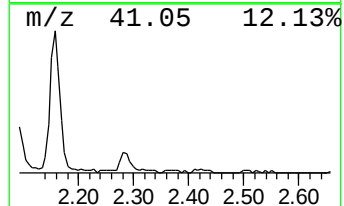
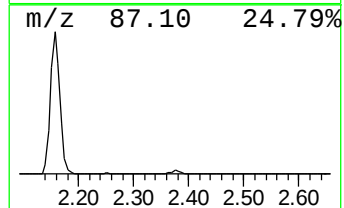
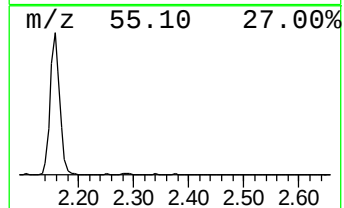
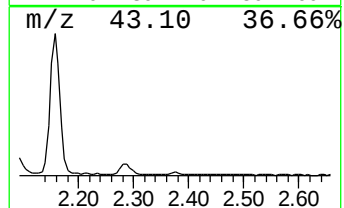
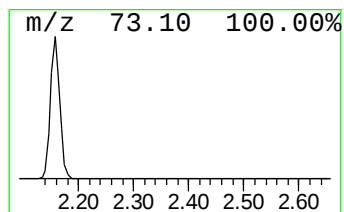
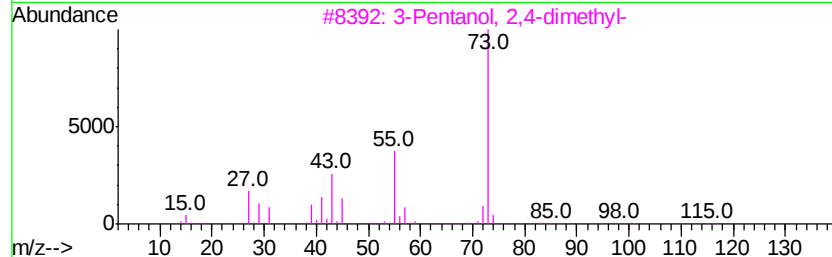
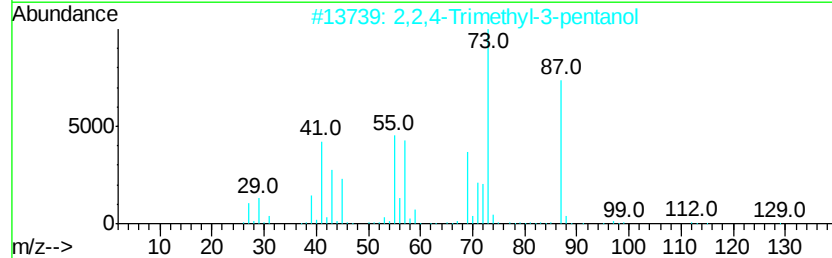
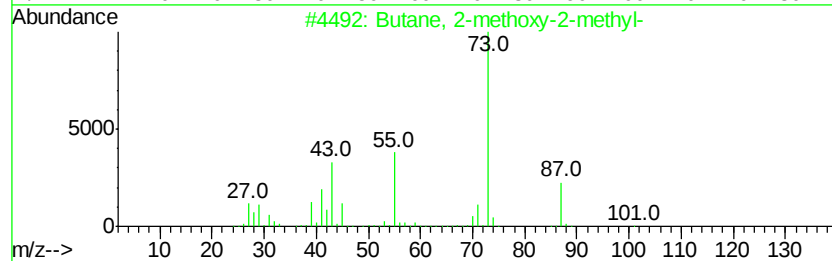
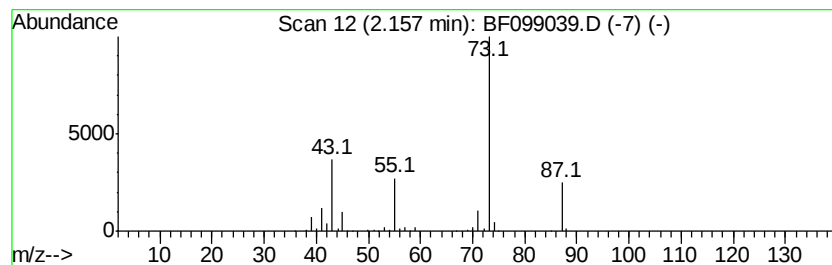
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	17.42 ng	632186	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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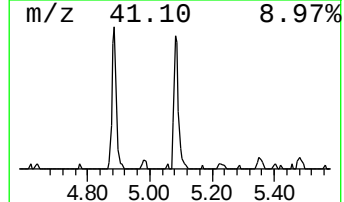
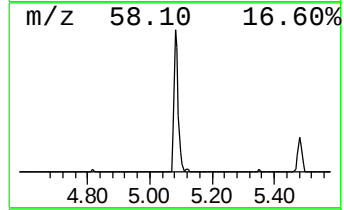
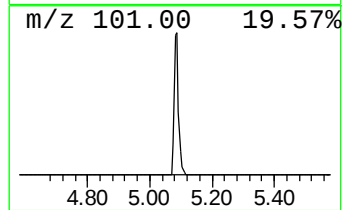
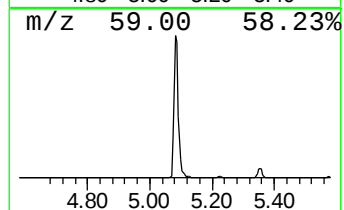
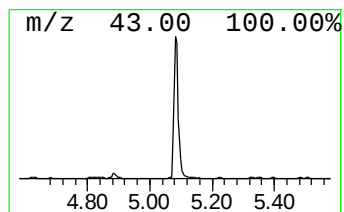
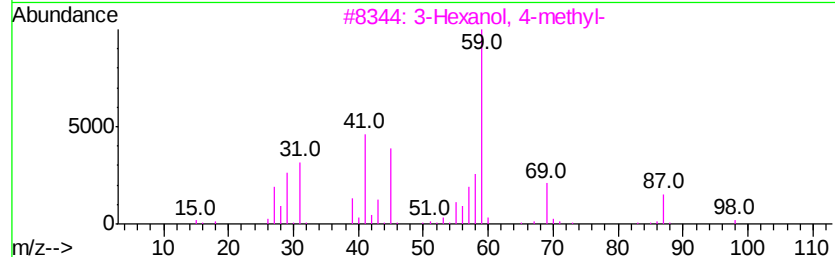
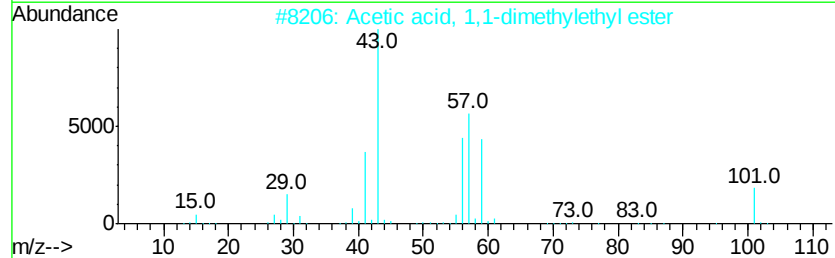
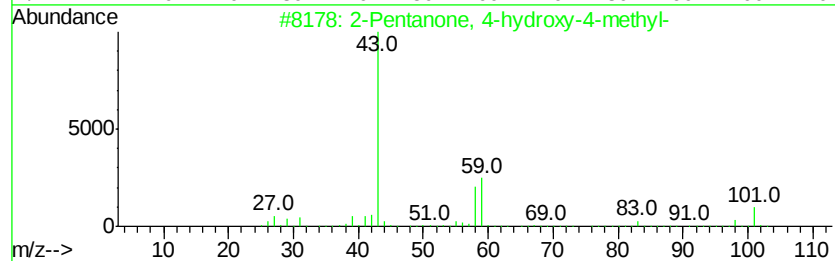
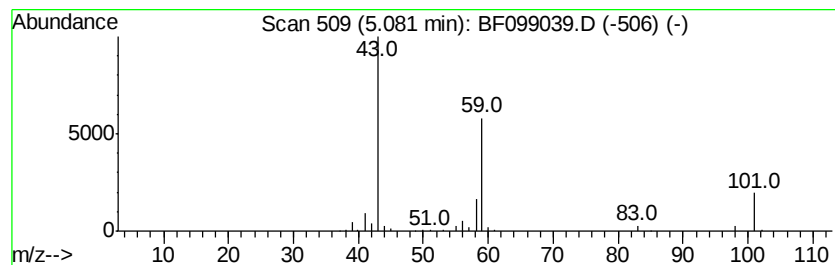
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	7.20 ng	261130	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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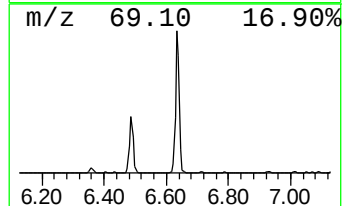
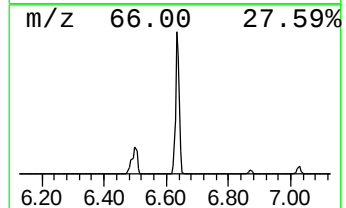
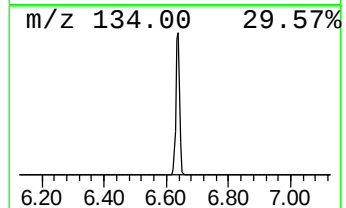
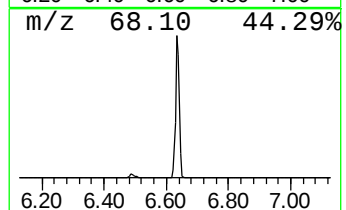
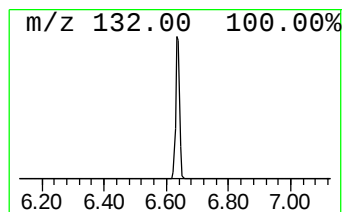
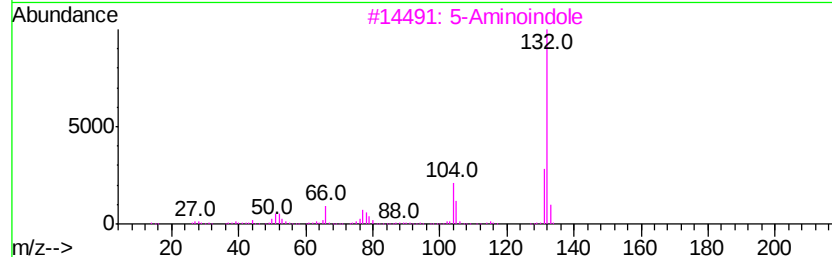
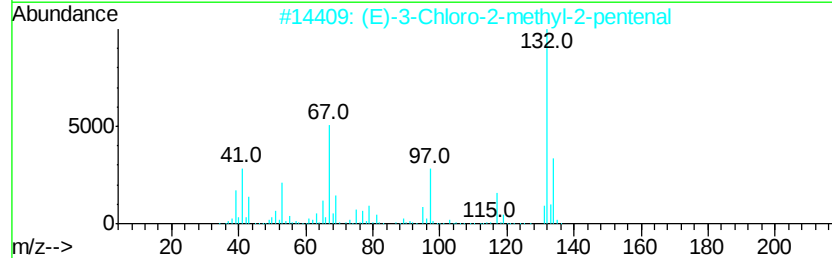
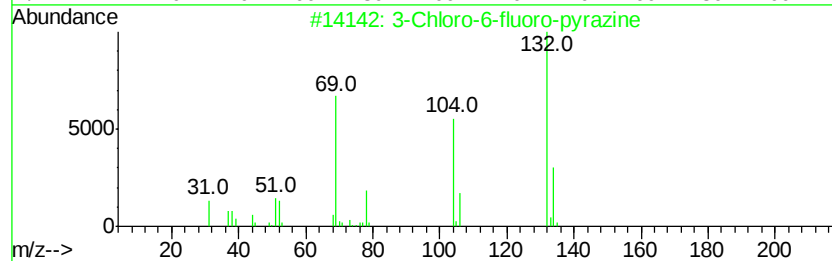
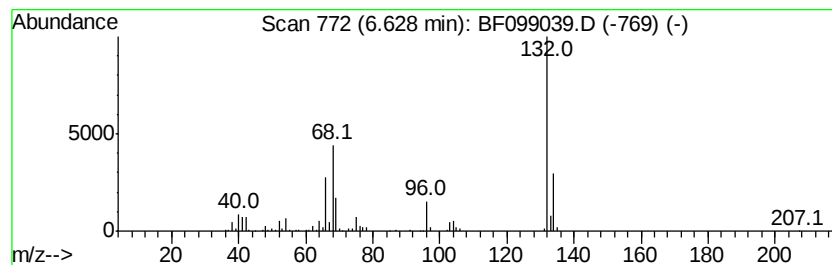
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	27.90 ng	1012390	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Amphetaminil	250	C17H18N2	017590-01-1	10



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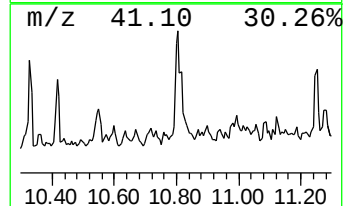
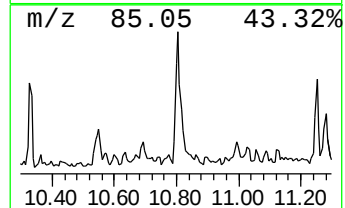
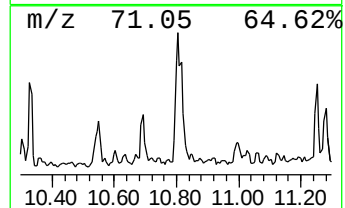
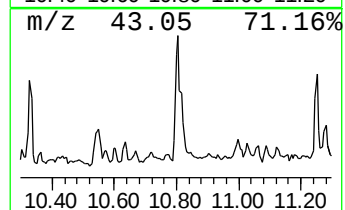
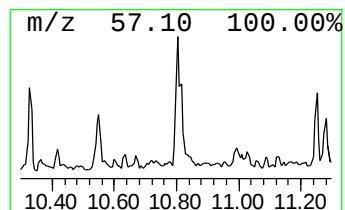
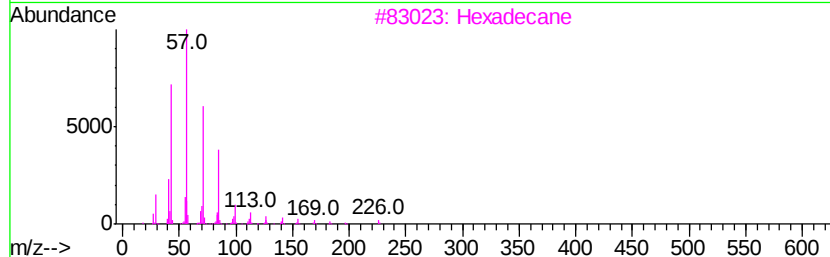
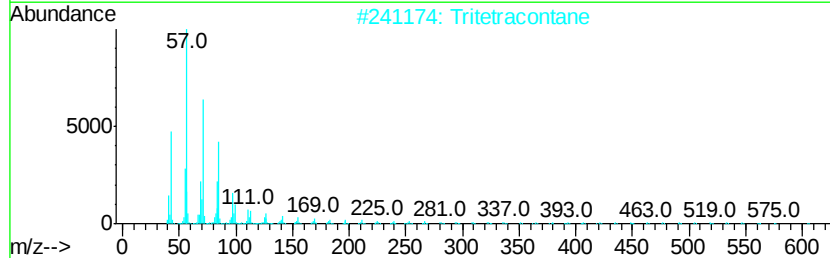
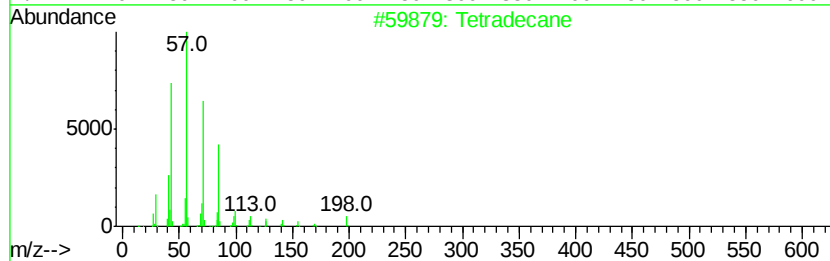
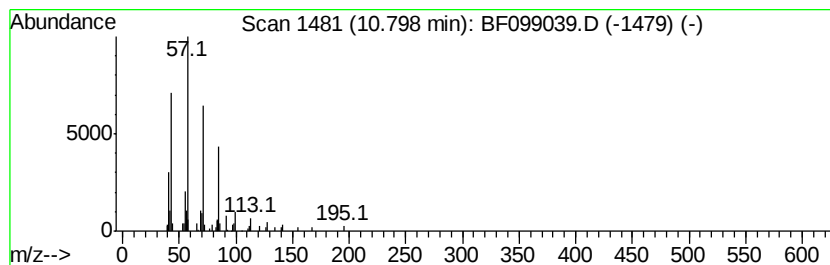
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	2.43 ng	130263	Phenanthrene-d10	11.39

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	91
2		Tritetracontane	605	C43H88	007098-21-7	90
3		Hexadecane	226	C16H34	000544-76-3	90
4		Tridecane	184	C13H28	000629-50-5	90
5		Heptadecane	240	C17H36	000629-78-7	90



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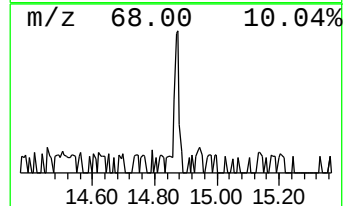
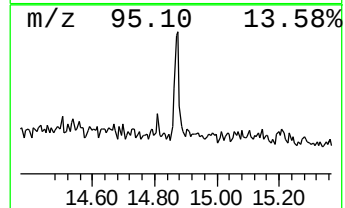
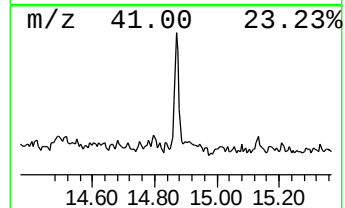
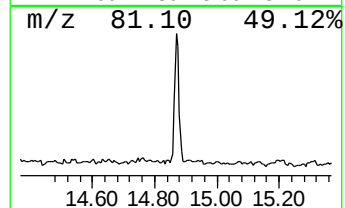
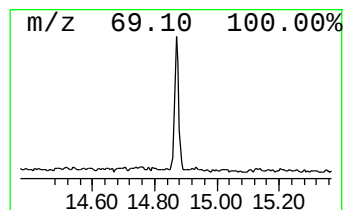
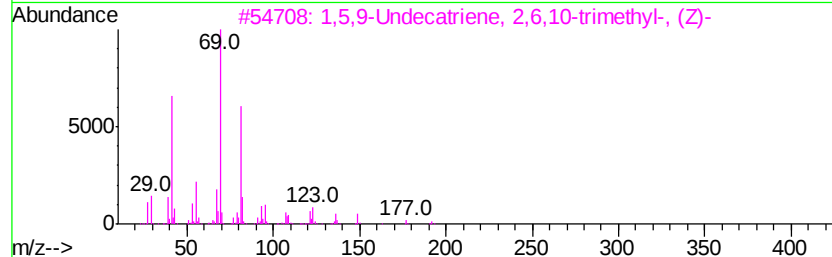
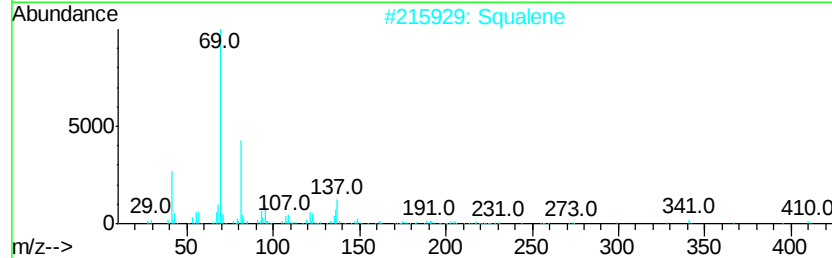
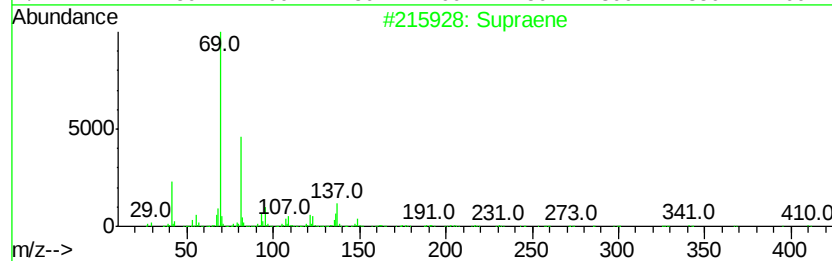
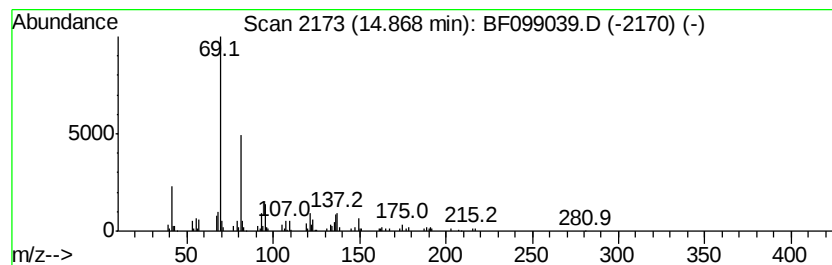
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	3.77 ng	106935	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	83
4		trans-Farnesol	222	C15H26O	000106-28-5	59
5		2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100317\
Data File : BF099039.D
Acq On : 3 Oct 2017 19:25
Operator : SJ/JU
Sample : I5496-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAMT-COMP-B

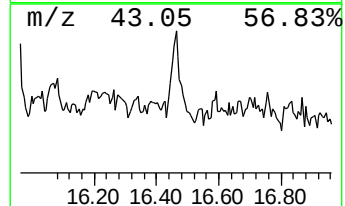
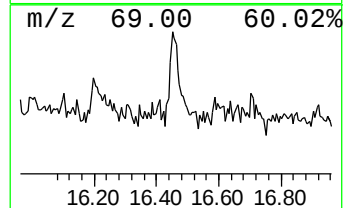
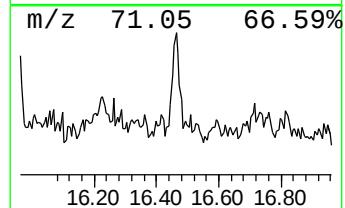
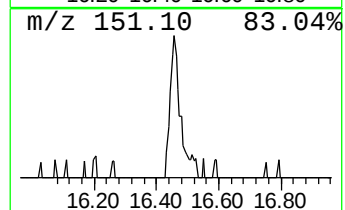
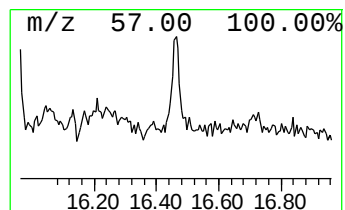
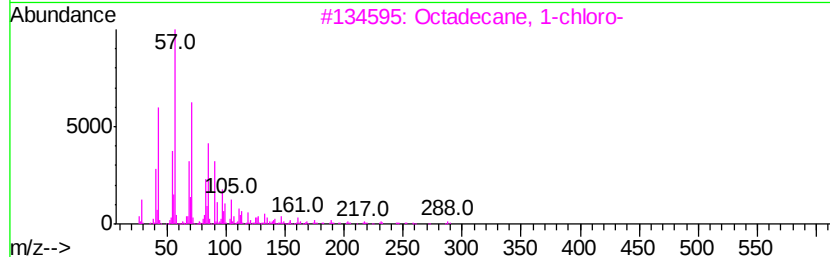
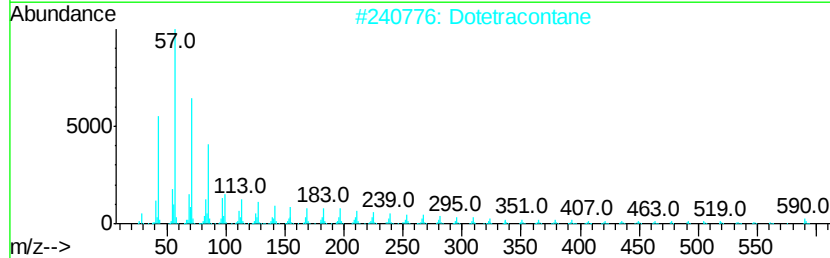
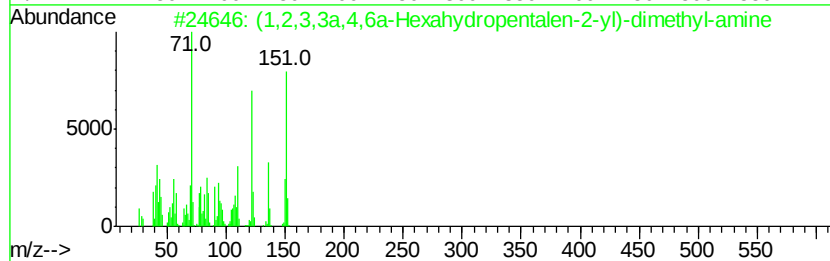
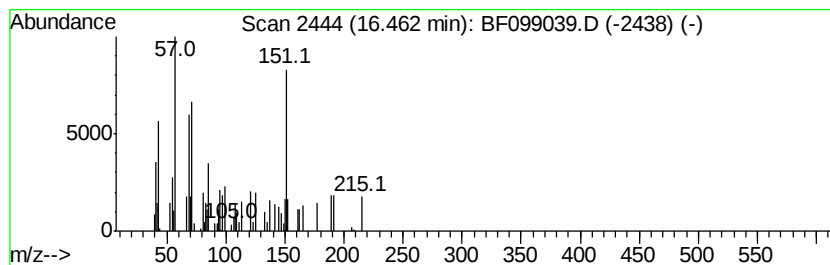
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.46 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.46	2.34 ng	66392	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(1,2,3,3a,4,6a-Hexahydropentalen...	151	C10H17N	031824-29-0	43
2		Dotetracontane	591	C42H86	007098-20-6	22
3		Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	22
4		Heneicosane	296	C21H44	000629-94-7	14
5		Tridecane, 2-methyl-	198	C14H30	001560-96-9	14



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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAMT-COMP-B

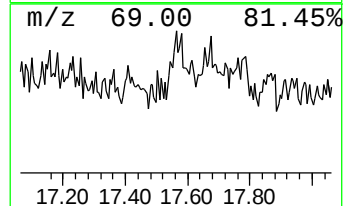
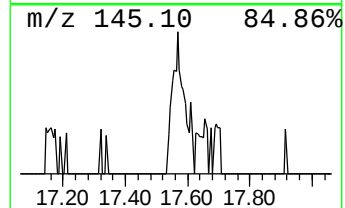
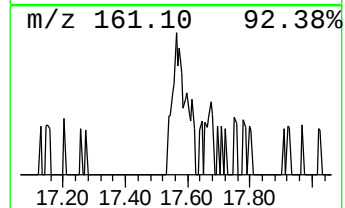
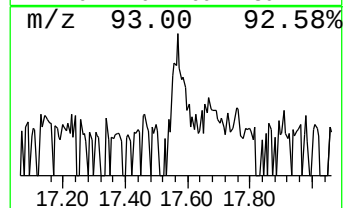
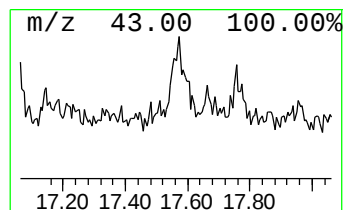
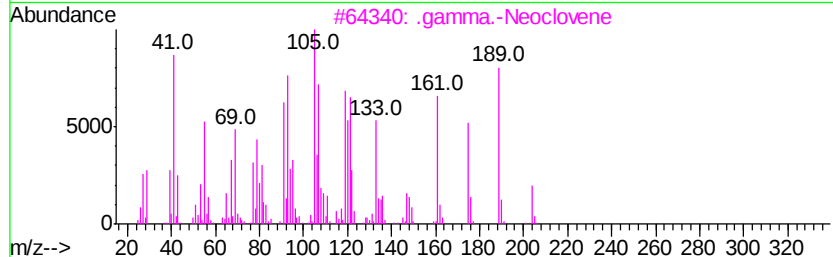
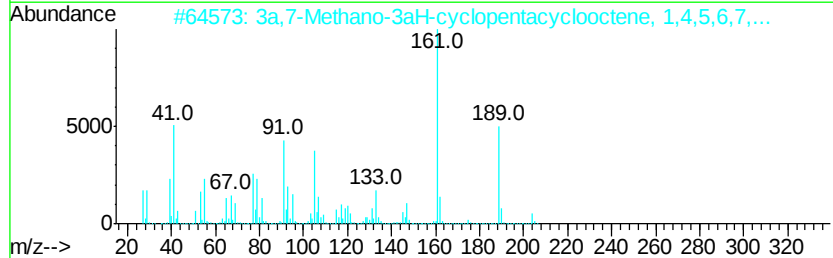
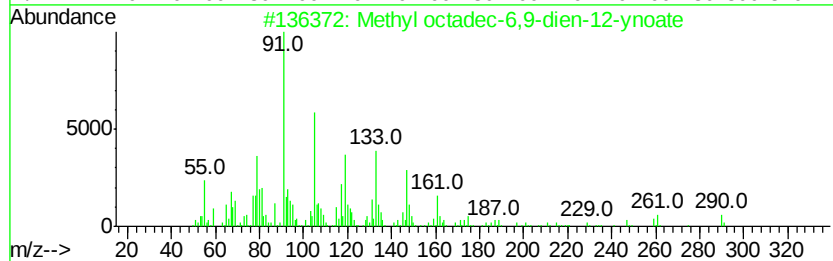
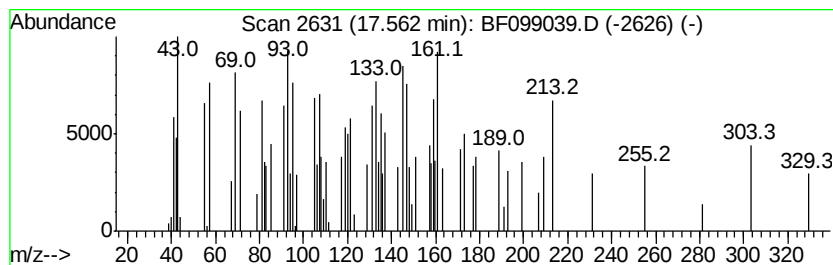
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown17.56 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.56	2.91 ng	82544	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl octadec-6,9-dien-12-ynoate	290	C19H30O2	1000336-42-0	14
2		3a,7-Methano-3aH-cyclopentacyclo...	204	C15H24	000469-92-1	12
3		.gamma.-Neoclovene	204	C15H24	1000156-11-7	12
4		.beta.-Panasinsene	204	C15H24	1000159-39-0	12
5		1H-Indole-2-carboxylic acid, 6-f...	193	C10H8FN02	1000362-66-5	10



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Sample : I5496-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAMT-COMP-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	2.16	17.4	ng	632186	1	6.87	725765	20.0
2-Pentanone, 4-hy...	5.08	7.2	ng	261130	1	6.87	725765	20.0
unknown6.63	6.63	27.9	ng	1012390	1	6.87	725765	20.0
Tetradecane	10.80	2.4	ng	130263	4	11.39	1070330	20.0
Supraene	14.87	3.8	ng	106935	6	15.50	567810	20.0
unknown16.46	16.46	2.3	ng	66392	6	15.50	567810	20.0
unknown17.56	17.56	2.9	ng	82544	6	15.50	567810	20.0