

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042718\
 Data File : BF104893.D
 Acq On : 27 Apr 2018 20:39
 Operator : JU/SJ
 Sample : J2161-09
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

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-BF040618.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	5.004	492	496	504	rBV	52512	71137	3.72%	0.403%
2	5.422	563	567	580	rBV	1621164	1728309	90.29%	9.784%
3	6.445	737	741	759	rBV	1614371	1736585	90.73%	9.831%
4	6.575	759	763	766	rBV	2015960	1777637	92.87%	10.063%
5	6.798	797	801	805	rBV	699671	557409	29.12%	3.155%
6	6.951	824	827	831	rBV	1479133	1376259	71.90%	7.791%
7	7.363	893	897	908	rBV	1102331	1057224	55.23%	5.985%
8	8.080	1016	1019	1032	rBV	736794	727944	38.03%	4.121%
9	9.157	1198	1202	1212	rBV	2253894	1914100	100.00%	10.835%
10	9.551	1265	1269	1277	rVB	111601	113255	5.92%	0.641%
11	9.763	1299	1305	1309	rBV	54633	51994	2.72%	0.294%
12	9.839	1314	1318	1327	rVB	858080	749313	39.15%	4.242%
13	10.257	1382	1389	1392	rBV2	90757	110564	5.78%	0.626%
14	10.480	1420	1427	1429	rBV2	25900	35551	1.86%	0.201%
15	10.633	1449	1453	1463	rBV	1120915	1041021	54.39%	5.893%
16	10.733	1468	1470	1477	rVB	71469	85208	4.45%	0.482%
17	11.180	1544	1546	1549	rBV	47455	42332	2.21%	0.240%
18	11.210	1549	1551	1554	rVV	37557	28238	1.48%	0.160%
19	11.333	1568	1572	1575	rBV	663587	658258	34.39%	3.726%
20	11.610	1617	1619	1623	rVB	46419	32852	1.72%	0.186%
21	11.851	1656	1660	1667	rBV2	185809	203264	10.62%	1.151%
22	12.016	1686	1688	1692	rBV	45318	46126	2.41%	0.261%
23	12.168	1711	1714	1721	rVB8	15817	27041	1.41%	0.153%
24	12.257	1727	1729	1734	rVB3	26601	31424	1.64%	0.178%
25	12.310	1734	1738	1740	rBV4	21875	29855	1.56%	0.169%
26	12.410	1752	1755	1759	rVB	53784	51962	2.71%	0.294%
27	12.504	1769	1771	1776	rVB3	20677	23001	1.20%	0.130%
28	12.545	1776	1778	1782	rBV	50200	64080	3.35%	0.363%
29	12.639	1791	1794	1798	rBV4	41958	51818	2.71%	0.293%
30	12.780	1815	1818	1824	rVB2	92365	90522	4.73%	0.512%
31	12.915	1837	1841	1845	rBV	1556253	1389214	72.58%	7.864%
32	13.139	1876	1879	1883	rBV2	54547	46686	2.44%	0.264%
33	13.480	1935	1937	1940	rBV	71452	57805	3.02%	0.327%
34	13.804	1989	1992	1995	rBV	182929	198049	10.35%	1.121%

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ALS Vial : 15 Sample Multiplier: 1

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-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

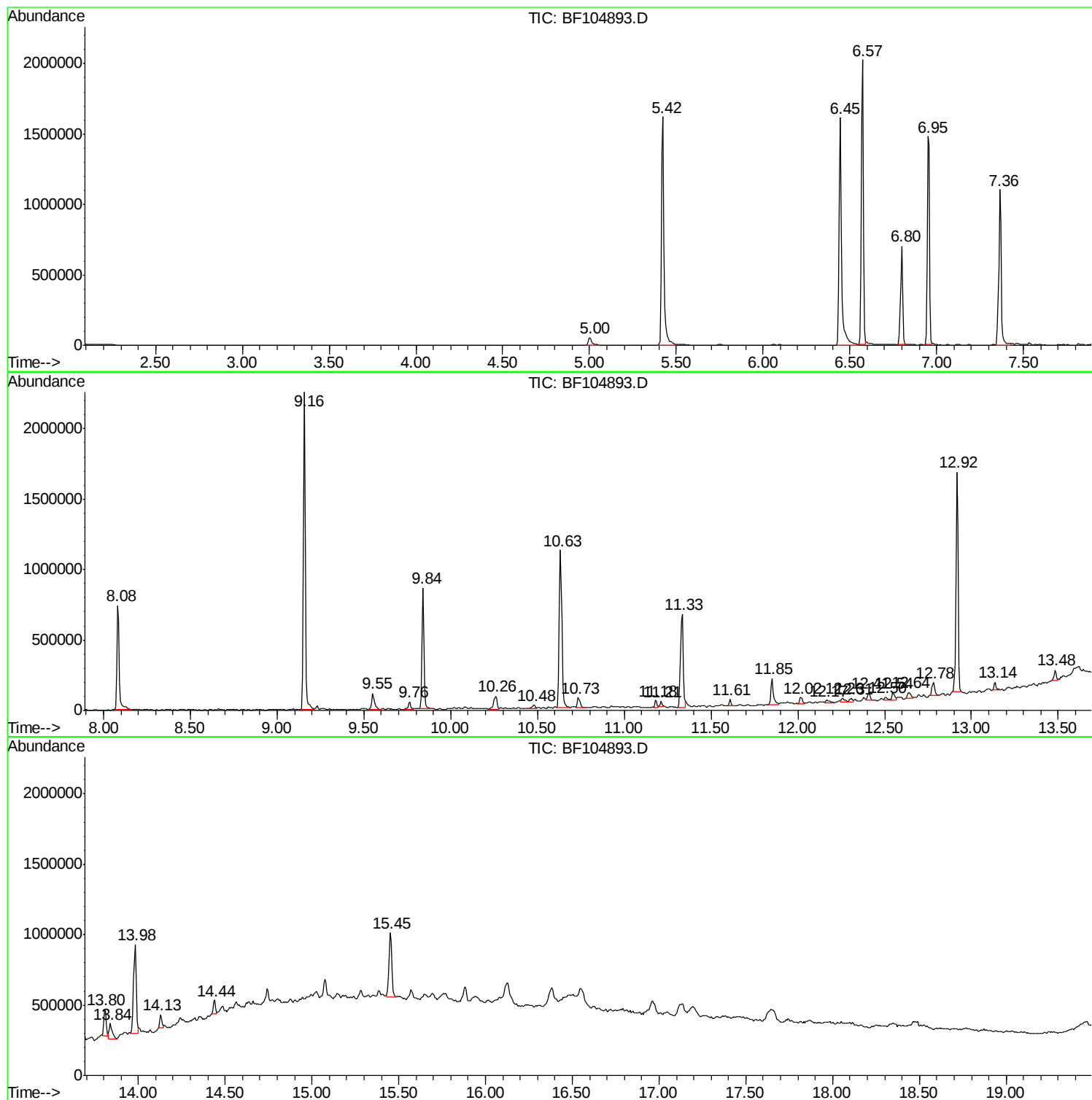
35	13.839	1996	1998	2004	rVB	106983	118838	6.21%	0.673%
36	13.980	2018	2022	2025	rBV	630958	583534	30.49%	3.303%
37	14.127	2045	2047	2050	rBV	95590	90013	4.70%	0.510%
38	14.439	2097	2100	2102	rBV	97829	93396	4.88%	0.529%
39	15.451	2268	2272	2278	rVB2	456662	573319	29.95%	3.245%

Sum of corrected areas: 17665137

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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.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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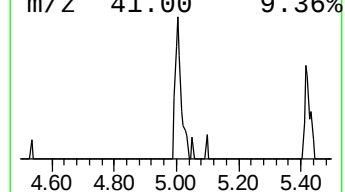
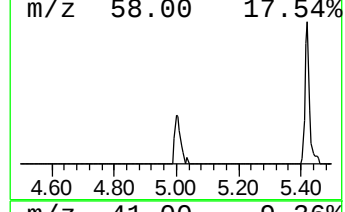
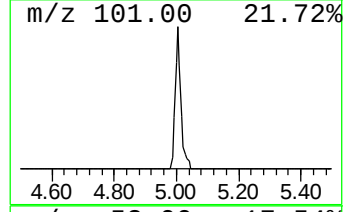
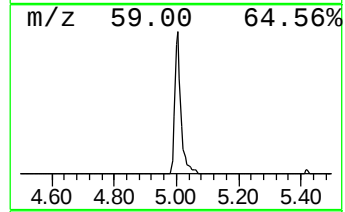
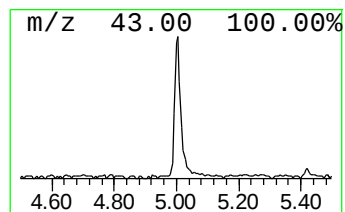
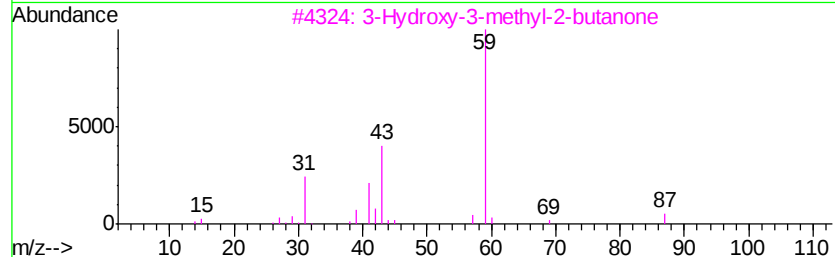
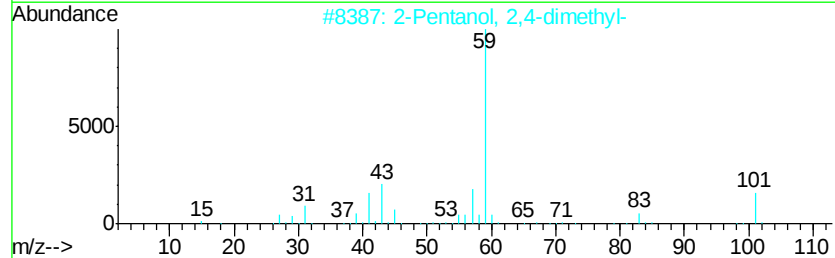
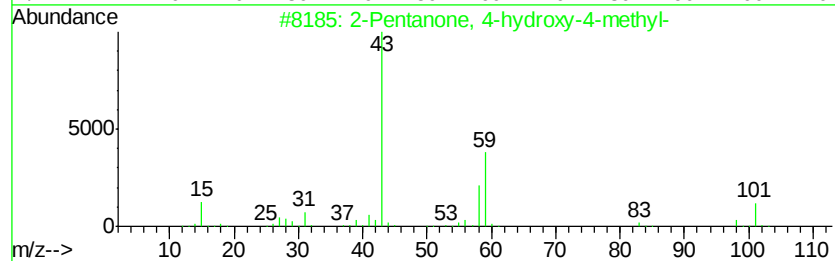
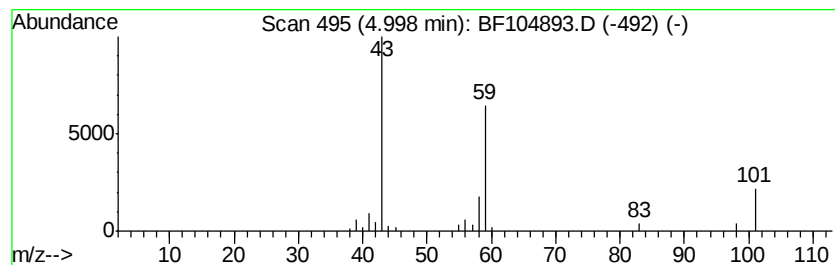
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	2.55 ng	71137	1,4-Dichlorobenzene-d4	6.80

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	38
3		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	35
4		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	28
5		3-Pentanol	88	C5H12O	000584-02-1	25



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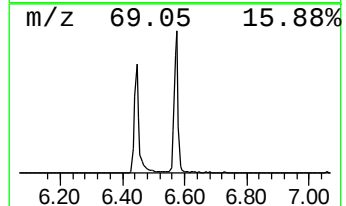
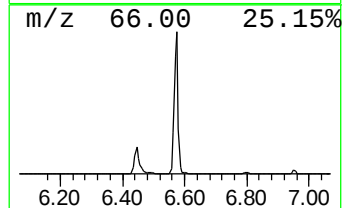
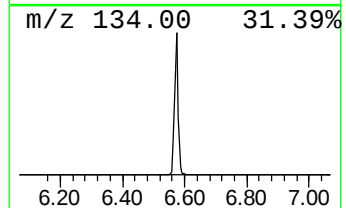
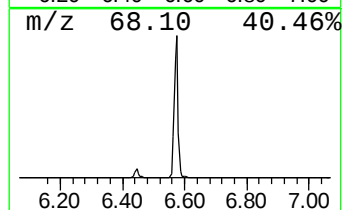
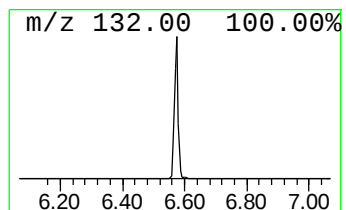
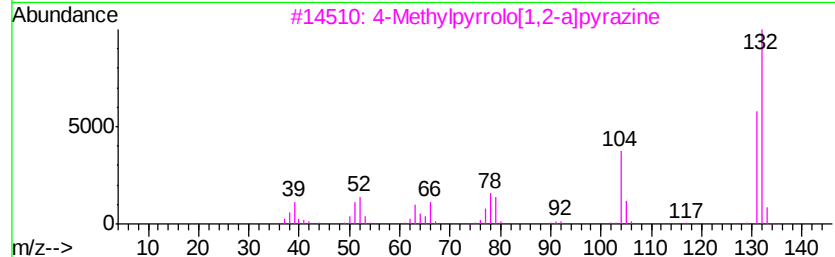
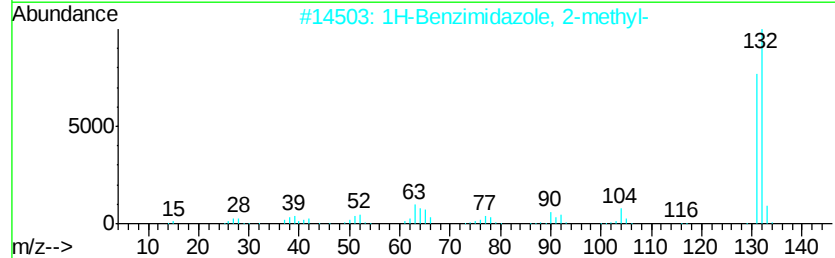
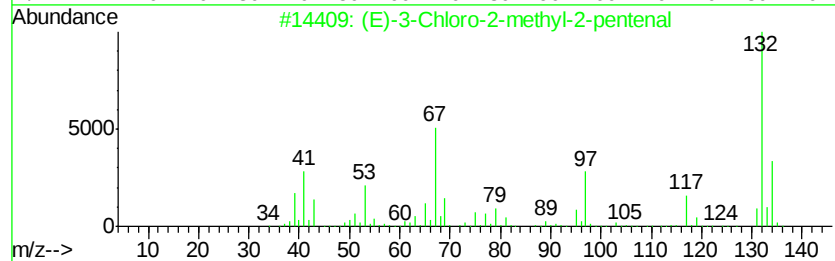
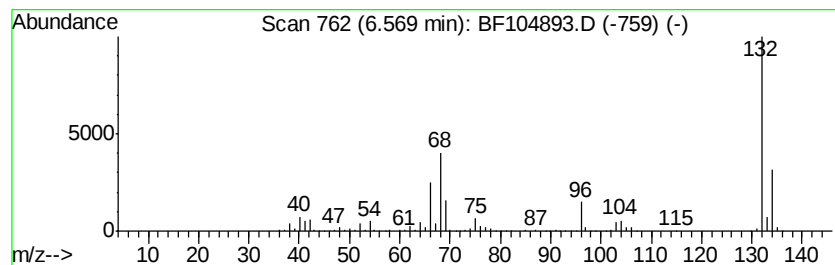
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	63.78 ng	1777640	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
3		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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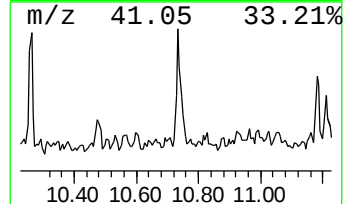
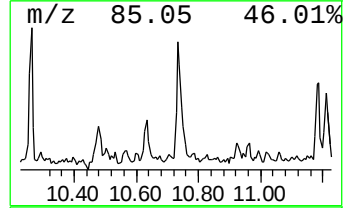
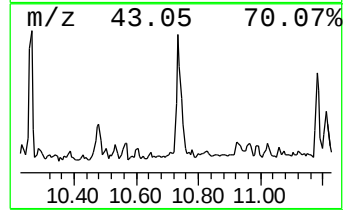
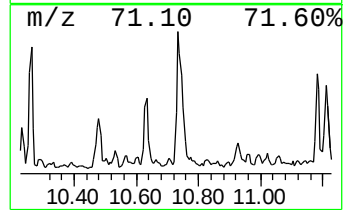
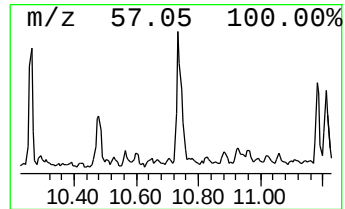
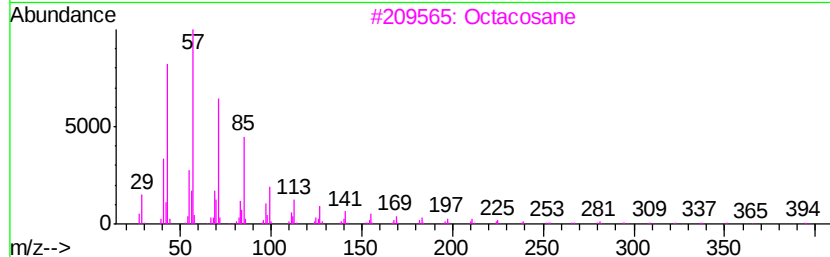
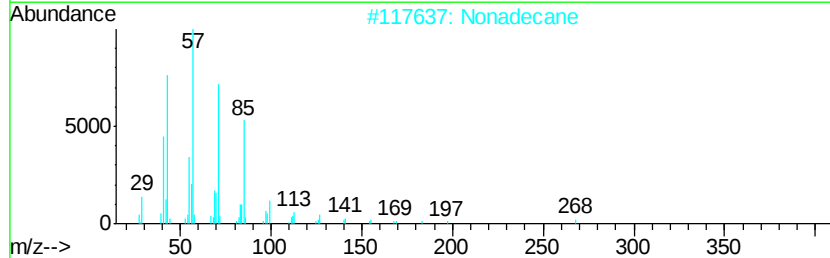
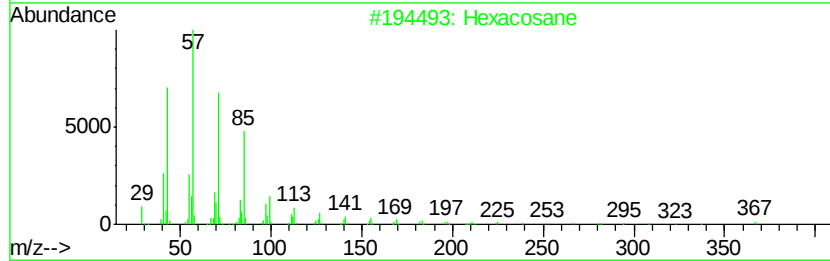
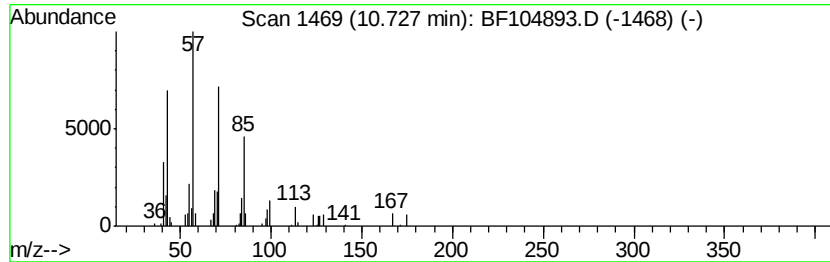
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Peak Number 5 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	2.59 ng	85208	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Nonadecane	268	C19H40	000629-92-5	90
3		Octacosane	394	C28H58	000630-02-4	90
4		Hexadecane	226	C16H34	000544-76-3	90
5		Heptadecane	240	C17H36	000629-78-7	90



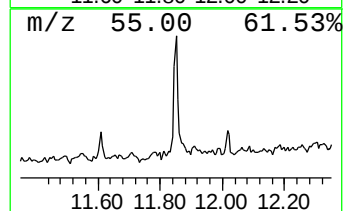
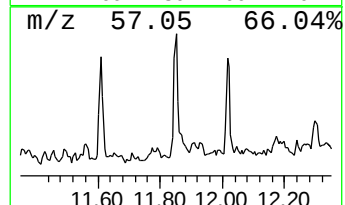
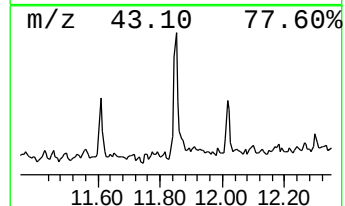
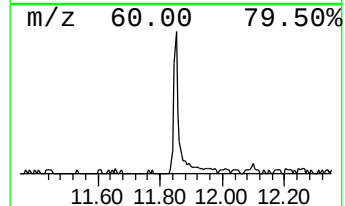
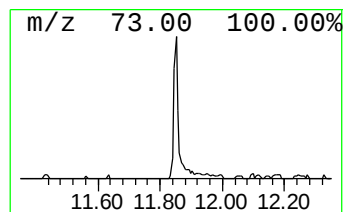
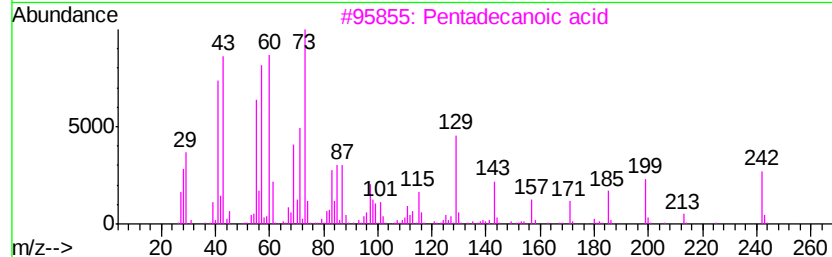
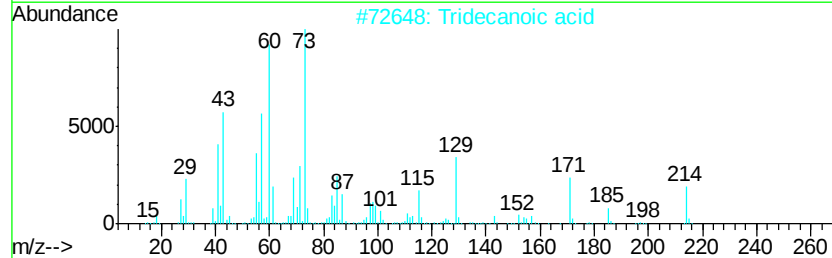
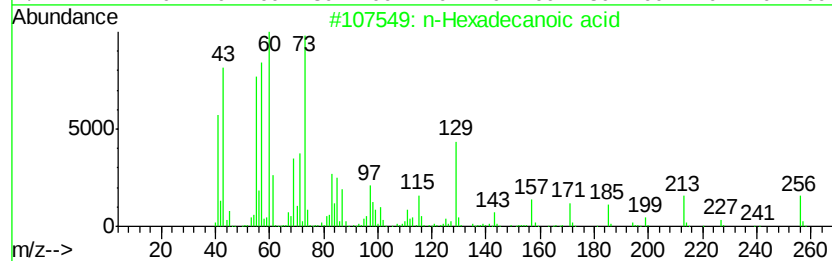
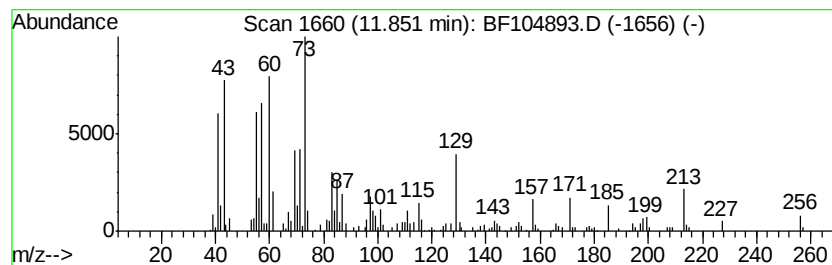
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TIC Library : C:\DATABASE\NIST11.L
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 Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.85	6.18 ng	203264	Phenanthrene-d10		11.33
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	81



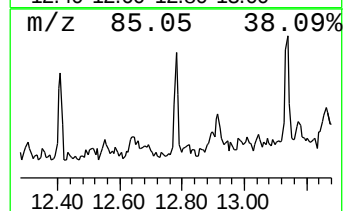
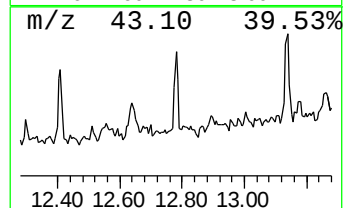
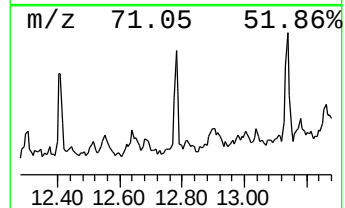
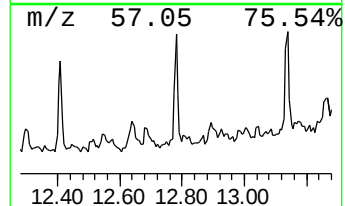
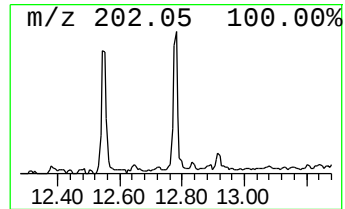
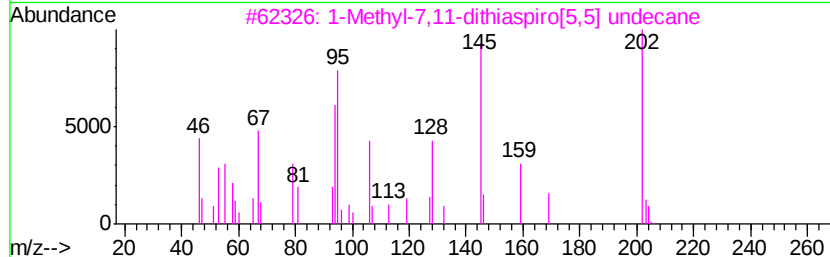
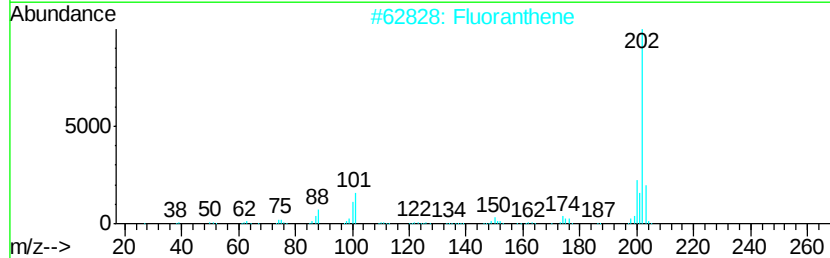
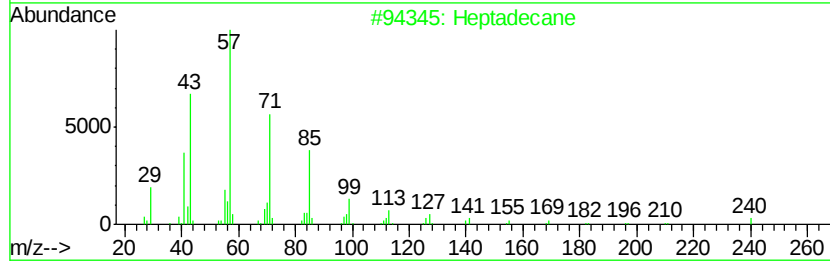
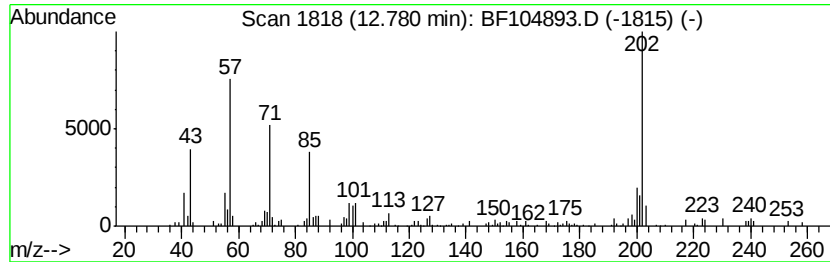
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Peak Number 7 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.78	3.10 ng	90522	Chrysene-d12		13.98	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	91
2		Fluoranthene	202	C16H10	000206-44-0	38
3		1-Methyl-7,11-dithiaspiro[5.5] u...	202	C10H18S2	107678-22-8	38
4		7H-Furo[3,2-g][1]benzopyran-7-on...	202	C11H6O4	002009-24-7	38
5		2-Naphthoic acid, 6-methoxy-	202	C12H10O3	002471-70-7	30



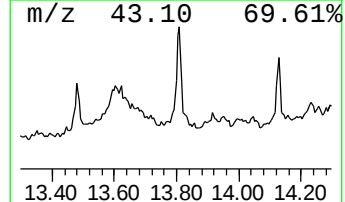
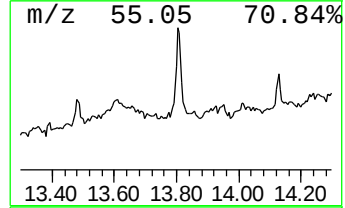
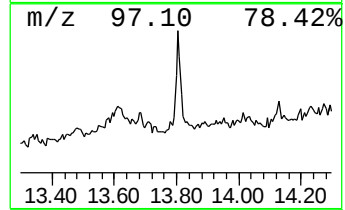
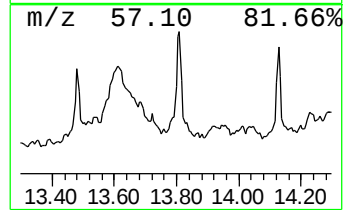
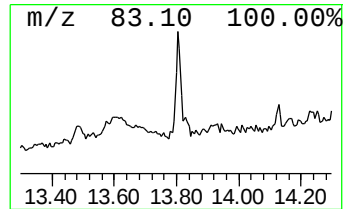
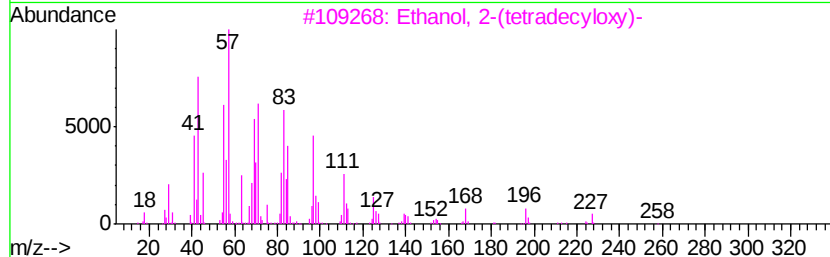
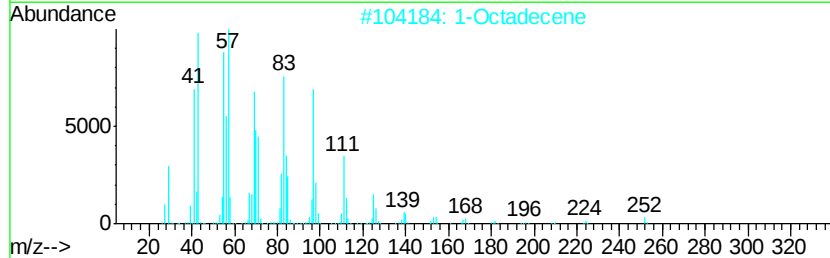
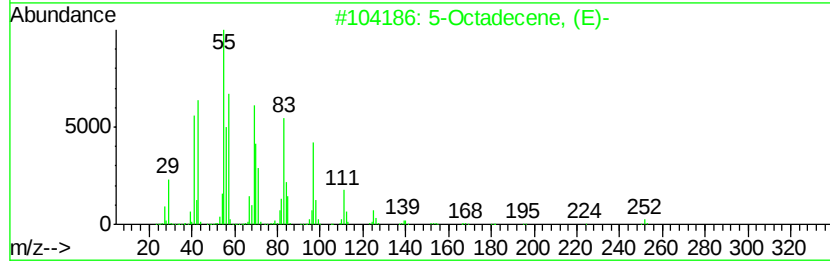
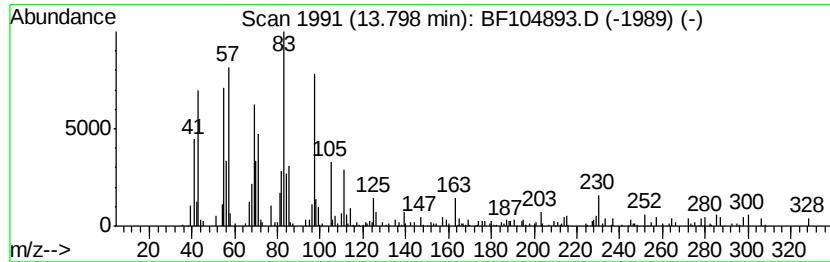
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Acq On : 27 Apr 2018 20:39
Operator : JU/SJ
Sample : J2161-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 5-Octadecene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.80	6.79 ng	198049	Chrysene-d12	13.98	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	97
2	1-Octadecene	252	C18H36	000112-88-9	95
3	Ethanol, 2-(tetradecyl)-	258	C16H34O2	002136-70-1	90
4	3-Octadecene, (E)-	252	C18H36	007206-19-1	86
5	5-Fluoro-3-trifluoromethylbenzoi...	474	C27H42F4O2	1000338-91-1	81



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104893.D
Acq On : 27 Apr 2018 20:39
Operator : JU/SJ
Sample : J2161-09
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ALS Vial : 15 Sample Multiplier: 1

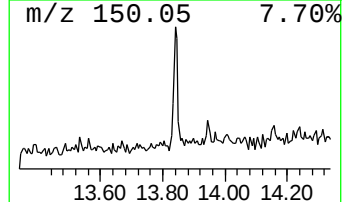
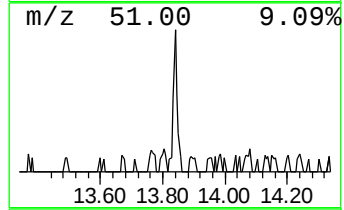
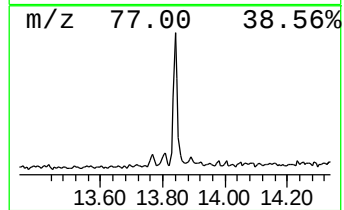
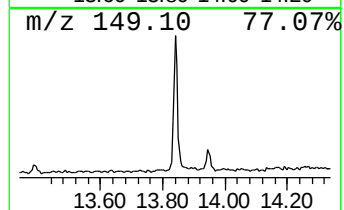
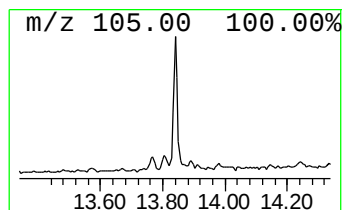
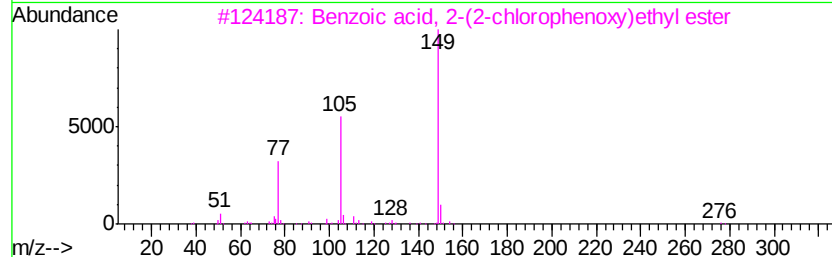
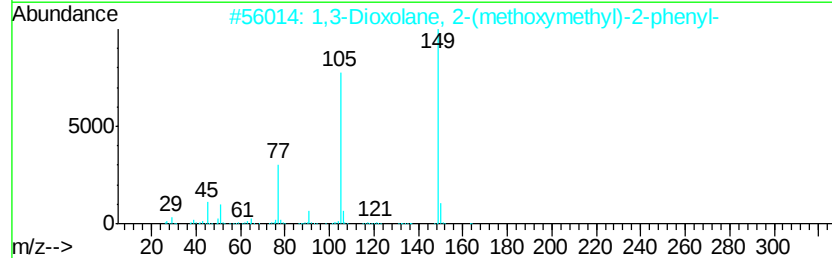
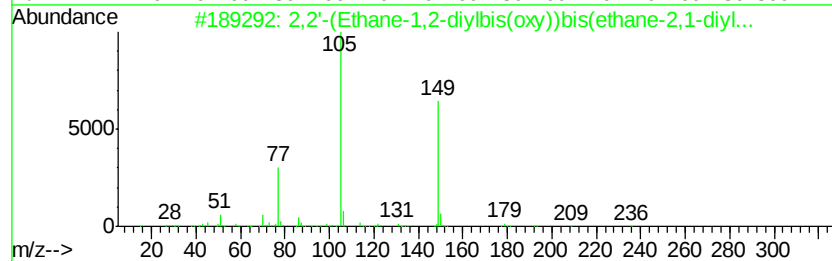
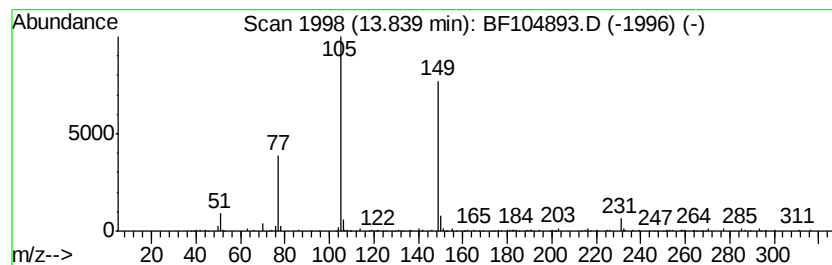
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2,2'-(Ethane-1,2-diylbis(ox... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	4.07 ng	118838	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,2'-(Ethane-1,2-diylbis(oxv))bi...	358	C20H22O6	1000366-99-4	78
2		1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59
3		Benzoic acid, 2-(2-chlorophenoxv...	276	C15H13ClO3	1000368-25-9	59
4		2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	50
5		2,3-Dimethyl-4a,8a-diphenyl-hexa...	326	C20H22O4	1000297-07-0	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
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Acq On : 27 Apr 2018 20:39
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Sample : J2161-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

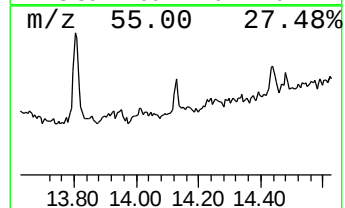
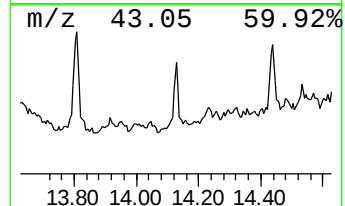
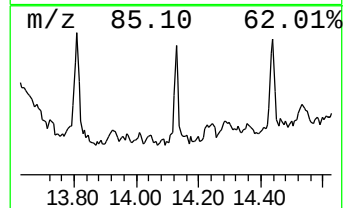
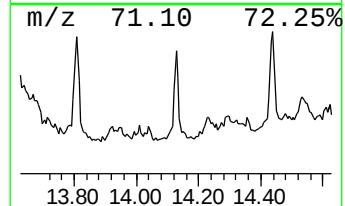
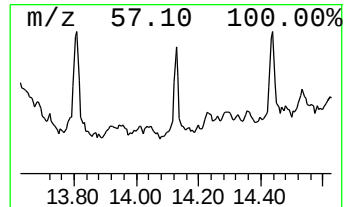
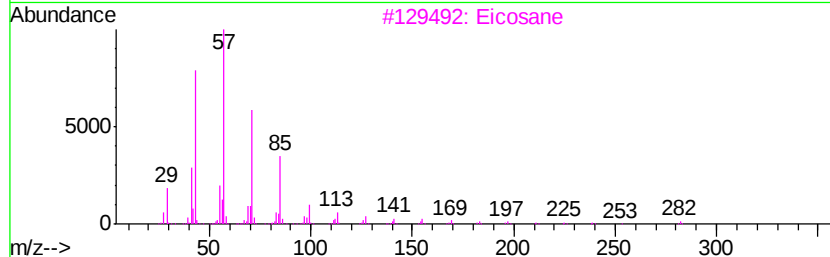
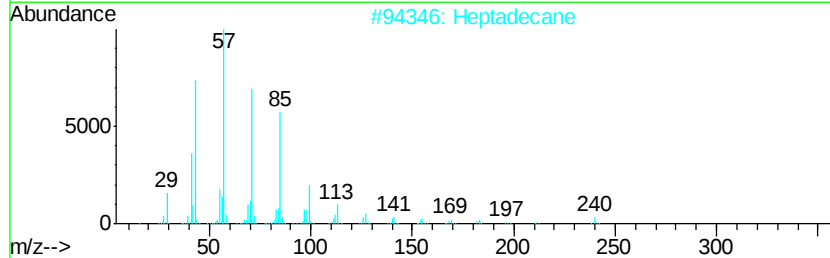
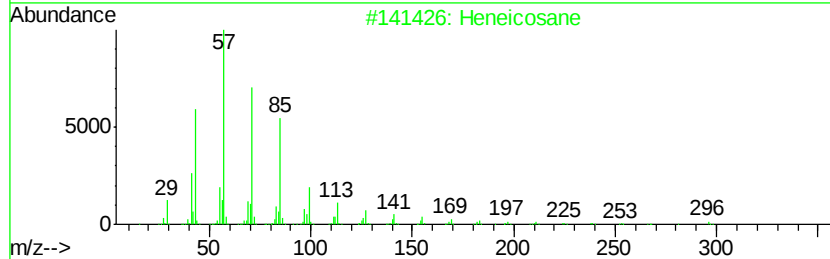
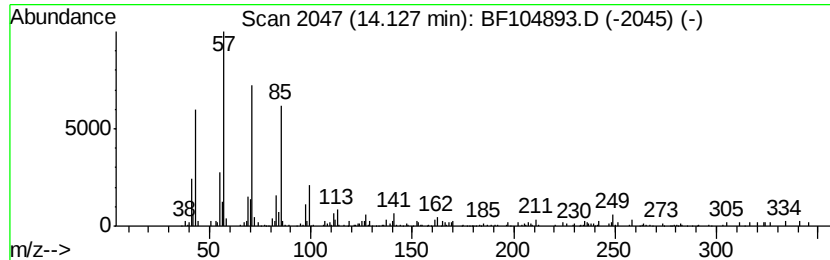
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	3.09 ng	90013	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	86
2		Heptadecane	240	C17H36	000629-78-7	86
3		Eicosane	282	C20H42	000112-95-8	86
4		Hexacosane	366	C26H54	000630-01-3	74
5		Nonadecane	268	C19H40	000629-92-5	72



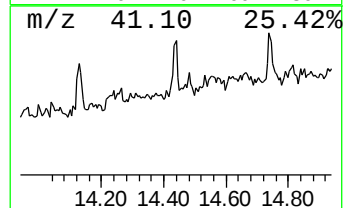
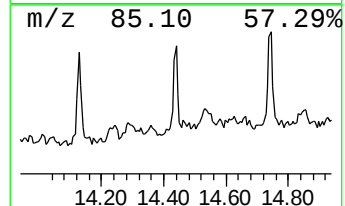
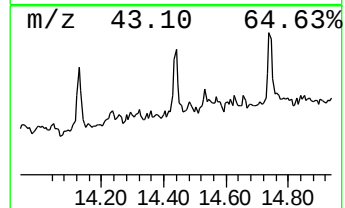
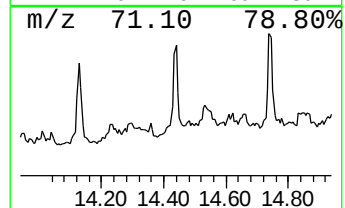
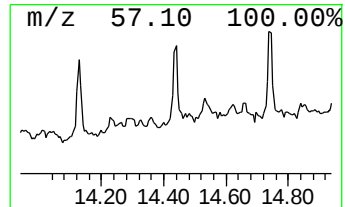
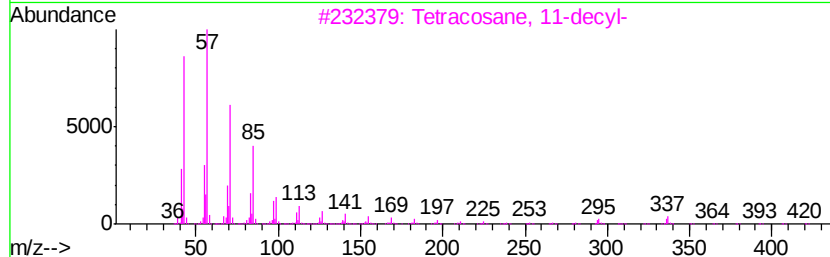
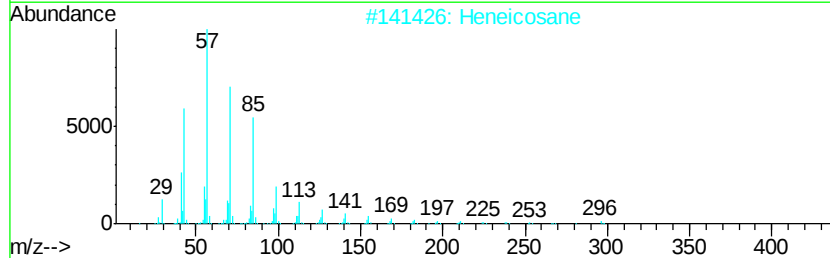
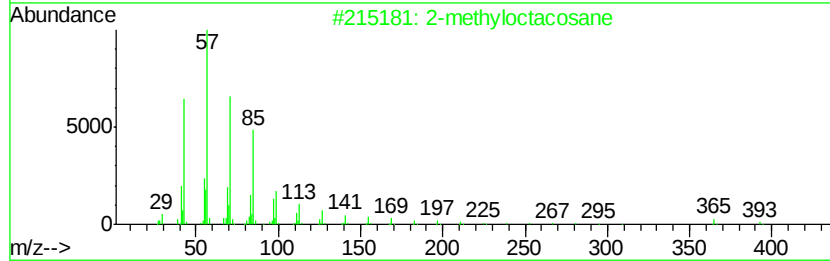
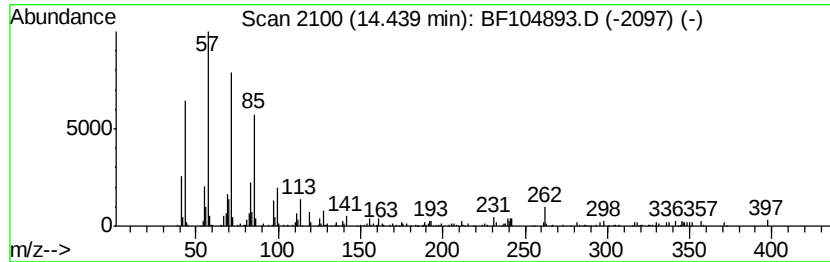
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Acq On : 27 Apr 2018 20:39
Operator : JU/SJ
Sample : J2161-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
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 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.44	3.20 ng	93396	Chrysene-d12	13.98	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	87
2	Heneicosane	296	C21H44	000629-94-7	87
3	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87
4	Hexacosane	366	C26H54	000630-01-3	83
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042718\
Data File : BF104893.D
Acq On : 27 Apr 2018 20:39
Operator : JU/SJ
Sample : J2161-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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...	5.00	2.5	ng	71137	1	6.80	557409	20.0
unknown6.57	6.57	63.8	ng	1777640	1	6.80	557409	20.0
Hexacosane	10.73	2.6	ng	85208	4	11.33	658258	20.0
n-Hexadecanoic acid	11.85	6.2	ng	203264	4	11.33	658258	20.0
Heptadecane	12.78	3.1	ng	90522	5	13.98	583534	20.0
5-Octadecene, (E)-	13.80	6.8	ng	198049	5	13.98	583534	20.0
2,2'-(Ethane-1,2-...	13.84	4.1	ng	118838	5	13.98	583534	20.0
Heneicosane	14.13	3.1	ng	90013	5	13.98	583534	20.0
2-methyloctacosane	14.44	3.2	ng	93396	5	13.98	583534	20.0